



wwPDB X-ray Structure Validation Summary Report

Feb 14, 2017 – 11:44 pm GMT

PDB ID : 1IVO
Title : Crystal Structure of the Complex of Human Epidermal Growth Factor and Receptor Extracellular Domains.
Authors : Ogiso, H.; Ishitani, R.; Nureki, O.; Fukai, S.; Yamanaka, M.; Kim, J.H.; Saito, K.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-03-28
Resolution : 3.30 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

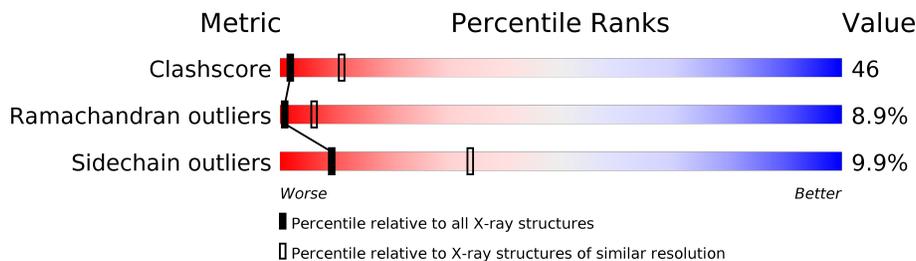
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)

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	622	
1	B	622	
2	C	53	
2	D	53	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1328	-	-	X	-
3	NAG	B	1328	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8892 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.

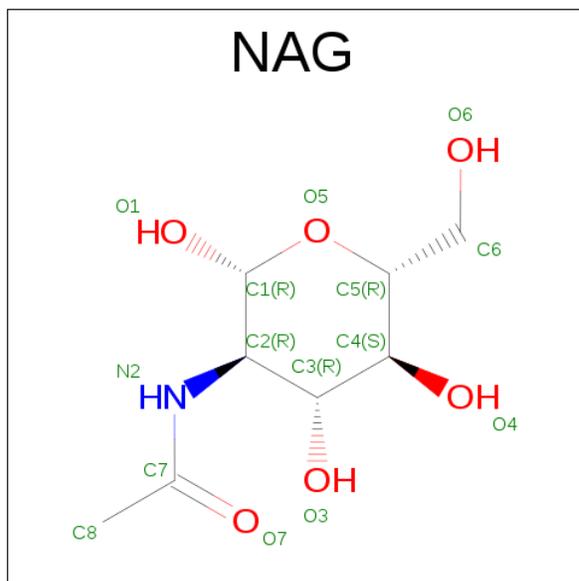
- Molecule 1 is a protein called Epidermal Growth Factor Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	511	Total 3956	C 2446	N 706	O 760	S 44	111	0	0
1	B	510	Total 3947	C 2441	N 705	O 757	S 44	62	0	0

- Molecule 2 is a protein called Epidermal growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	47	Total 385	C 244	N 63	O 71	S 7	0	0	0
2	D	47	Total 385	C 244	N 63	O 71	S 7	0	0	0

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



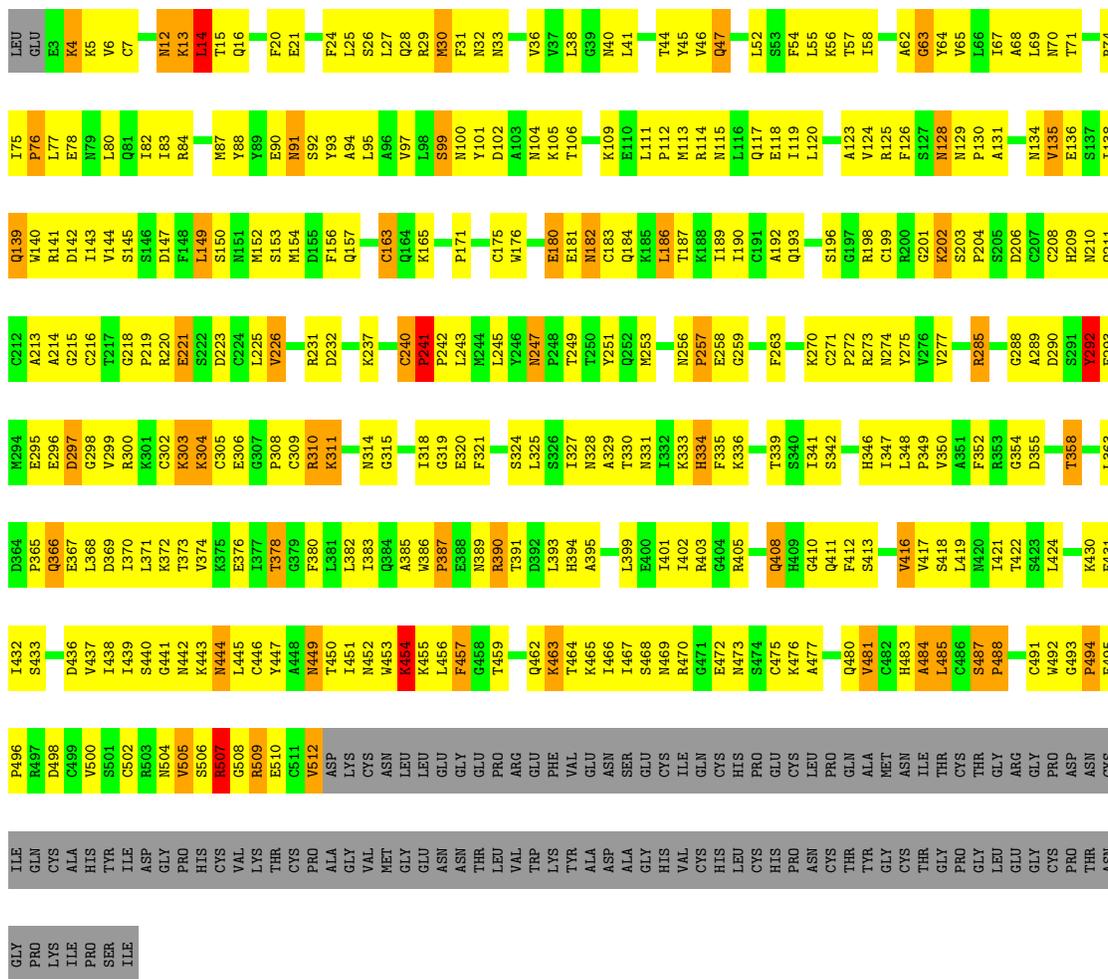
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	32	Total	O	0	0
			32	32		
5	C	6	Total	O	0	0
			6	6		
5	D	6	Total	O	0	0
			6	6		



• Molecule 2: Epidermal growth factor



• Molecule 2: Epidermal growth factor



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	220.16Å 220.16Å 113.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.30	Depositor
% Data completeness (in resolution range)	98.0 (10.00-3.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.255 , 0.326	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8892	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.33	0/4027	0.67	1/5438 (0.0%)
1	B	0.34	0/4018	0.67	1/5426 (0.0%)
2	C	0.36	0/396	0.64	0/536
2	D	0.35	0/396	0.63	0/536
All	All	0.34	0/8837	0.67	2/11936 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	CYS	CA-CB-SG	-5.07	104.87	114.00
1	B	240	CYS	CA-CB-SG	-5.06	104.90	114.00

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	3956	0	3843	342	0
1	B	3947	0	3843	397	0
2	C	385	0	344	22	0
2	D	385	0	344	42	0
3	A	70	0	65	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	0	39	21	0
4	A	28	0	25	4	0
5	A	35	0	0	2	0
5	B	32	0	0	5	0
5	C	6	0	0	1	0
5	D	6	0	0	2	0
All	All	8892	0	8503	788	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 46.

The worst 5 of 788 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:243:LEU:HA	1:B:256:ASN:HB3	1.34	1.09
1:A:174:SER:HB3	1:A:184:GLN:HB3	1.39	1.02
1:A:481:VAL:HG12	1:A:482:CYS:H	1.24	0.99
1:B:328:ASN:H	3:B:1328:NAG:H82	1.27	0.97
1:A:331:ASN:HB2	3:A:1328:NAG:HN2	1.29	0.96

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	509/622 (82%)	368 (72%)	93 (18%)	48 (9%)	1 5
1	B	508/622 (82%)	369 (73%)	98 (19%)	41 (8%)	1 7
2	C	45/53 (85%)	35 (78%)	9 (20%)	1 (2%)	8 37
2	D	45/53 (85%)	31 (69%)	6 (13%)	8 (18%)	0 1
All	All	1107/1350 (82%)	803 (72%)	206 (19%)	98 (9%)	1 6

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	14	LEU
1	A	146	SER
1	A	171	PRO
1	A	203	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	449/543 (83%)	408 (91%)	41 (9%)	11	38
1	B	448/543 (82%)	402 (90%)	46 (10%)	8	32
2	C	41/47 (87%)	37 (90%)	4 (10%)	9	34
2	D	41/47 (87%)	35 (85%)	6 (15%)	3	18
All	All	979/1180 (83%)	882 (90%)	97 (10%)	9	34

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	13	LYS
1	B	219	PRO
2	C	24	GLU
1	B	30	MET
1	B	139	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	28	GLN
1	B	128	ASN
1	B	469	ASN
1	B	47	GLN
1	A	252	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](#)

2 carbohydrates 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	$\# Z > 2$
4	NAG	A	1420	1,4	14,14,15	0.63	0	15,19,21	1.17	1 (6%)
4	NAG	A	2420	4	14,14,15	0.67	0	15,19,21	0.68	0

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
4	NAG	A	1420	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2420	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1420	NAG	C4-C3-C2	3.13	115.60	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1420	NAG	4	0
4	A	2420	NAG	3	0

5.6 Ligand geometry [i](#)

8 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
3	NAG	A	1032	1	14,14,15	0.58	0	15,19,21	0.67	0
3	NAG	A	1151	1	14,14,15	0.59	0	15,19,21	0.86	0
3	NAG	A	1172	1	14,14,15	0.59	0	15,19,21	0.71	0
3	NAG	A	1328	1	14,14,15	0.81	1 (7%)	15,19,21	1.00	1 (6%)
3	NAG	A	1337	1	14,14,15	0.54	0	15,19,21	0.58	0
3	NAG	B	1032	1	14,14,15	0.47	0	15,19,21	0.86	1 (6%)
3	NAG	B	1151	1	14,14,15	0.61	0	15,19,21	0.62	0
3	NAG	B	1328	1	14,14,15	0.74	0	15,19,21	1.00	0

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
3	NAG	A	1032	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1151	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1172	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1328	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1337	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1032	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1151	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1328	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1328	NAG	C1-C2	2.48	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1328	NAG	C3-C4-C5	-2.67	105.51	110.22
3	B	1032	NAG	C2-N2-C7	-2.22	119.70	122.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1172	NAG	C8-C7-N2-C2
3	A	1328	NAG	O7-C7-N2-C2
3	A	1172	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1328	NAG	8	0
3	A	1337	NAG	1	0
3	B	1032	NAG	1	0
3	B	1151	NAG	1	0
3	B	1328	NAG	19	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.