



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 09:47 AM UTC

PDB ID : 1IVO / pdb_00001ivo
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

<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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

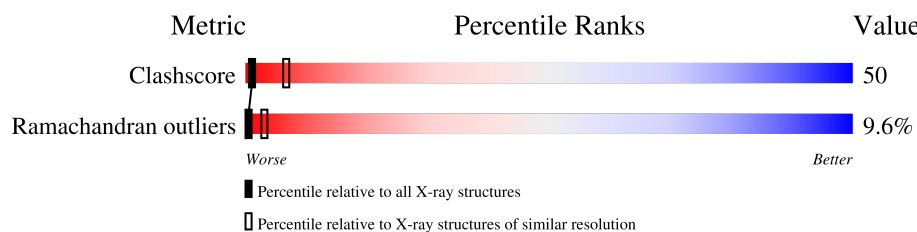
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	622	31% 44% 7% 18%
1	B	622	29% 48% 5% 18%
2	C	53	34% 51% • 11%
2	D	53	34% 51% • 11%
3	E	2	50% 50%

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
4	NAG	A	1328	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	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
1	A	511	Total	C	N	O	S	111	0	0
			3956	2446	706	760	44			
1	B	510	Total	C	N	O	S	62	0	0
			3947	2441	705	757	44			

- Molecule 2 is a protein called Epidermal growth factor.

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

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- 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		

Note EDS was not executed.

- [illegible]

- Chain B:  29% 48% 5% 18%



4 Data and refinement statistics

Xtriage (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	220.16 Å 220.16 Å 113.12 Å 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.	Xtriage
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	0.43	0/4027	1.06	26/5438 (0.5%)
1	B	0.41	0/4018	1.03	19/5426 (0.4%)
2	C	0.43	0/396	1.03	2/536 (0.4%)
2	D	0.41	0/396	1.01	3/536 (0.6%)
All	All	0.42	0/8837	1.04	50/11936 (0.4%)

There are no bond length outliers.

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	GLU	N-CA-C	-9.15	99.16	110.88
1	A	75	ILE	CA-C-N	8.68	130.68	119.84
1	A	75	ILE	C-N-CA	8.68	130.68	119.84
1	A	405	ARG	N-CA-C	-8.44	102.76	113.23
1	B	47	GLN	N-CA-C	8.29	121.22	110.53

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	371	0
1	B	3947	0	3843	429	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	385	0	344	28	0
2	D	385	0	344	43	0
3	E	28	0	25	4	0
4	A	70	0	65	10	0
4	B	42	0	39	22	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	852	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 50.

The worst 5 of 852 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	4:B:1328:NAG:H82	1.27	0.97
1:A:331:ASN:HB2	4:A:1328:NAG:HN2	1.29	0.96

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	378/622 (61%)	270 (71%)	69 (18%)	39 (10%)	0 2
1	B	307/622 (49%)	225 (73%)	55 (18%)	27 (9%)	0 4
All	All	685/1244 (55%)	495 (72%)	124 (18%)	66 (10%)	0 3

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	PRO
1	A	203	SER
1	A	310	ARG
1	A	311	LYS
1	A	427	ARG

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides 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	E	1	3,1	14,14,15	0.65	0	17,19,21	1.11	1 (5%)
3	NAG	E	2	3	14,14,15	0.70	0	17,19,21	0.67	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	E	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	5/6/23/26	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(°)
3	E	1	NAG	C4-C3-C2	3.13	115.60	111.02

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

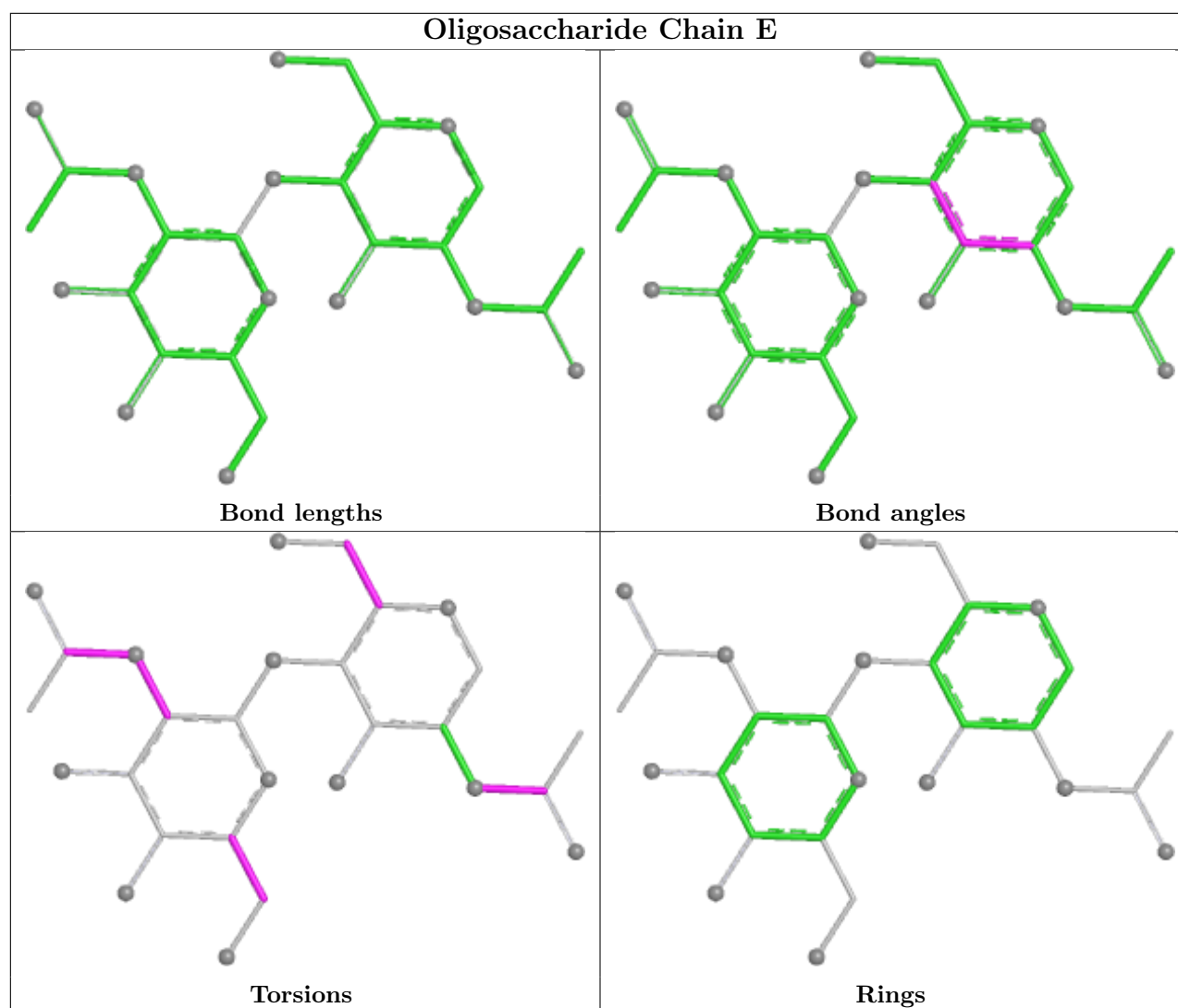
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	4	0
3	E	2	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



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	$\# Z > 2$
4	NAG	A	1032	1	14,14,15	0.60	0	17,19,21	0.66	0
4	NAG	A	1337	1	14,14,15	0.56	0	17,19,21	0.56	0
4	NAG	B	1151	1	14,14,15	0.64	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1328	1	14,14,15	0.84	1 (7%)	17,19,21	0.96	1 (5%)
4	NAG	A	1151	1	14,14,15	0.62	0	17,19,21	0.83	1 (5%)
4	NAG	B	1032	1	14,14,15	0.50	0	17,19,21	0.82	1 (5%)
4	NAG	A	1172	1	14,14,15	0.62	0	17,19,21	0.68	0
4	NAG	B	1328	1	14,14,15	0.76	0	17,19,21	0.99	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	1032	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1337	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1151	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1328	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1151	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1032	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1172	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1328	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1328	NAG	C1-C2	2.59	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1328	NAG	C3-C4-C5	-2.61	105.51	110.23
4	B	1032	NAG	C2-N2-C7	-2.39	119.70	122.90
4	A	1151	NAG	C2-N2-C7	-2.02	120.19	122.90

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1032	NAG	C3-C2-N2-C7
4	A	1032	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	A	1032	NAG	O7-C7-N2-C2
4	A	1151	NAG	C8-C7-N2-C2
4	A	1151	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1337	NAG	1	0
4	B	1151	NAG	1	0
4	A	1328	NAG	9	0
4	B	1032	NAG	1	0
4	B	1328	NAG	20	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.