



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:49 PM UTC

PDB ID : 1AXI / pdb_00001axi
Title : STRUCTURAL PLASTICITY AT THE HGH:HGHBP INTERFACE
Authors : Atwell, S.; Ultsch, M.; De Vos, A.M.; Wells, J.A.
Deposited on : 1997-10-15
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

<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

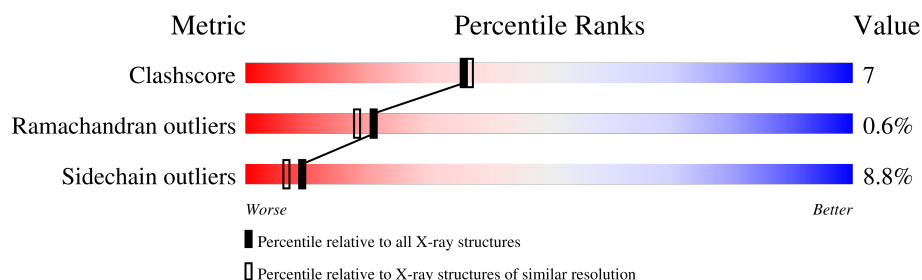
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 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	191	 63% 24% 5% • 8%
2	B	236	 61% 16% 5% 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3321 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 GROWTH HORMONE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1396	897	237	255	7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	ARG	GLY	engineered mutation	UNP P01241
A	129	THR	GLU	conflict	UNP P01241
A	168	ARG	LYS	engineered mutation	UNP P01241
A	171	THR	ASP	engineered mutation	UNP P01241
A	172	TYR	LYS	engineered mutation	UNP P01241
A	174	ALA	GLU	engineered mutation	UNP P01241
A	176	TYR	PHE	engineered mutation	UNP P01241

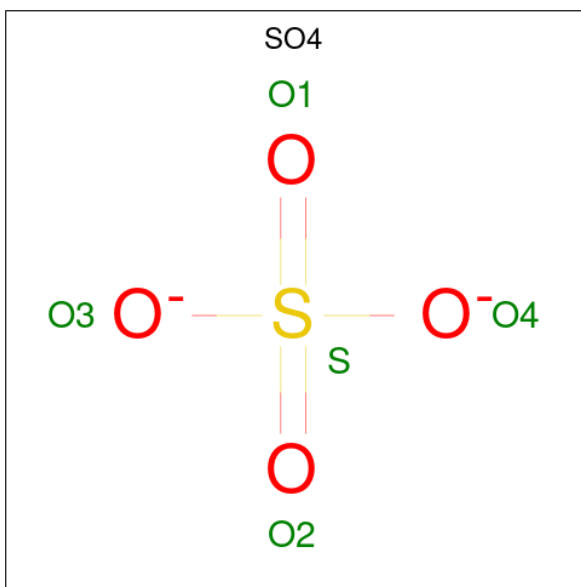
- Molecule 2 is a protein called GROWTH HORMONE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	191	Total	C	N	O	S	0	0	0
			1538	983	256	289	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	31	GLY	LYS	conflict	UNP P10912
B	61	GLU	LEU	conflict	UNP P10912
B	104	ALA	TRP	engineered mutation	UNP P10912

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O	0	0
			127	127		
4	B	255	Total	O	0	0
			255	255		

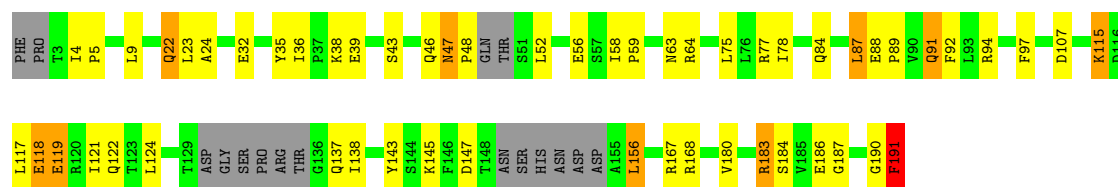
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

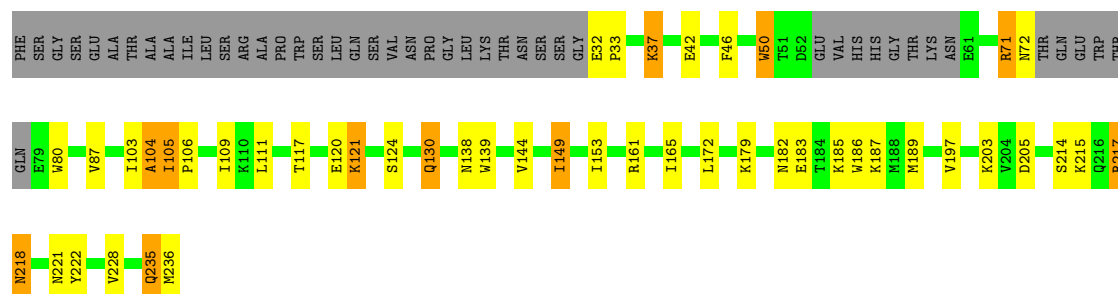
• Molecule 1: GROWTH HORMONE

Chain A: 



• Molecule 2: GROWTH HORMONE RECEPTOR

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	65.60Å 65.60Å 231.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC, X-PLOR	Depositor
R, R_{free}	0.190 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3321	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: SO4

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	0.82	0/1422	1.77	20/1921 (1.0%)
2	B	0.89	0/1578	1.82	26/2145 (1.2%)
All	All	0.86	0/3000	1.80	46/4066 (1.1%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	87	VAL	CB-CA-C	-13.24	96.18	111.80
1	A	58	ILE	CA-C-O	10.05	125.08	119.15
1	A	191	PHE	CA-CB-CG	8.91	122.71	113.80
2	B	121	LYS	CA-CB-CG	7.98	130.05	114.10
1	A	59	PRO	CB-CA-C	7.82	118.51	111.40
2	B	46	PHE	CA-CB-CG	7.65	121.45	113.80
2	B	235	GLN	OE1-CD-NE2	-7.33	115.27	122.60
2	B	87	VAL	N-CA-C	7.23	118.54	111.67
2	B	218	ASN	CA-CB-CG	-7.11	105.49	112.60
1	A	22	GLN	OE1-CD-NE2	6.92	129.52	122.60
1	A	97	PHE	CA-CB-CG	6.83	120.63	113.80
1	A	118	GLU	CB-CG-CD	6.82	124.19	112.60
2	B	104	ALA	CA-C-O	-6.57	111.11	120.51
2	B	37	LYS	N-CA-C	6.43	118.63	108.79
2	B	217	ARG	NE-CZ-NH2	-6.38	113.45	119.20
2	B	138	ASN	CA-C-O	-6.20	114.63	121.33
2	B	124	SER	CA-CB-OG	-6.18	98.73	111.10
2	B	80	TRP	N-CA-C	6.13	119.50	109.76
1	A	92	PHE	CA-CB-CG	-6.11	107.69	113.80
2	B	117	THR	CA-C-O	-6.03	113.50	120.49
2	B	186	TRP	CA-C-O	-5.92	114.23	120.80
1	A	32	GLU	CA-C-N	5.81	128.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	GLU	C-N-CA	5.81	128.06	120.28
1	A	77	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	A	63	ASN	CA-CB-CG	-5.75	106.85	112.60
2	B	182	ASN	CA-CB-CG	-5.69	106.91	112.60
2	B	205	ASP	N-CA-CB	-5.68	100.86	110.41
2	B	161	ARG	CA-C-O	-5.64	113.48	119.97
1	A	78	ILE	CA-C-O	-5.53	115.20	120.95
1	A	190	GLY	CA-C-N	5.46	131.52	121.70
1	A	190	GLY	C-N-CA	5.46	131.52	121.70
2	B	139	TRP	CA-C-O	-5.38	115.15	121.44
2	B	221	ASN	OD1-CG-ND2	5.32	127.92	122.60
1	A	184	SER	O-C-N	5.29	129.58	122.49
1	A	180	VAL	CA-C-O	-5.25	115.60	121.17
1	A	183	ARG	CG-CD-NE	5.24	123.54	112.00
1	A	121	ILE	N-CA-C	-5.24	105.61	110.53
2	B	153	ILE	O-C-N	-5.17	117.54	122.97
2	B	103	ILE	O-C-N	-5.16	116.07	122.52
2	B	218	ASN	CA-C-O	-5.14	114.25	120.32
1	A	119	GLU	CB-CG-CD	5.13	121.33	112.60
2	B	50	TRP	CA-C-O	-5.13	115.60	121.40
2	B	130	GLN	O-C-N	5.11	124.33	121.27
2	B	183	GLU	CG-CD-OE1	5.09	130.12	118.40
2	B	149	ILE	N-CA-C	-5.06	105.62	113.16
1	A	64	ARG	CD-NE-CZ	-5.03	117.35	124.40

There are no chirality outliers.

There are no planarity outliers.

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	1396	0	1351	22	0
2	B	1538	0	1474	23	0
3	B	5	0	0	0	0
4	A	127	0	0	4	0
4	B	255	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3321	0	2825	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 7.

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)
2:B:105:ILE:HG13	2:B:106:PRO:HD2	1.59	0.85
2:B:71:ARG:HB2	2:B:105:ILE:HD11	1.68	0.76
2:B:71:ARG:CB	2:B:105:ILE:HD11	2.21	0.70
1:A:183:ARG:HD3	4:A:250:HOH:O	1.92	0.70
2:B:109:ILE:HD11	2:B:121:LYS:HD3	1.77	0.67
1:A:168:ARG:HG3	2:B:104:ALA:HB1	1.79	0.64
1:A:91:GLN:HG3	1:A:107:ASP:OD2	1.98	0.63
1:A:187:GLY:HA2	4:A:304:HOH:O	1.98	0.62
1:A:84:GLN:HA	1:A:87:LEU:HD22	1.80	0.62
1:A:35:TYR:HB3	1:A:156:LEU:HD11	1.81	0.61
2:B:179:LYS:HA	2:B:187:LYS:HE3	1.81	0.61
1:A:46:GLN:NE2	2:B:120:GLU:OE2	2.36	0.59
1:A:52:LEU:HA	1:A:56:GLU:OE2	2.06	0.55
2:B:32:GLU:N	2:B:33:PRO:HD2	2.23	0.54
1:A:47:ASN:HD22	1:A:48:PRO:HD2	1.73	0.53
1:A:187:GLY:O	1:A:191:PHE:HD1	1.93	0.52
2:B:189:MET:HE1	2:B:197:VAL:HG21	1.92	0.51
2:B:37:LYS:NZ	2:B:130:GLN:HE22	2.09	0.50
1:A:143:TYR:CE1	1:A:145:LYS:HE3	2.47	0.49
2:B:32:GLU:N	2:B:33:PRO:CD	2.76	0.49
2:B:130:GLN:NE2	4:B:316:HOH:O	2.44	0.49
1:A:22:GLN:HG2	4:A:257:HOH:O	2.12	0.49
1:A:48:PRO:HB3	2:B:71:ARG:HG2	1.94	0.48
1:A:119:GLU:HA	1:A:122:GLN:HE21	1.79	0.48
1:A:47:ASN:HD22	1:A:48:PRO:CD	2.27	0.48
1:A:4:ILE:HG23	1:A:5:PRO:HD2	1.98	0.46
1:A:24:ALA:HB1	1:A:167:ARG:HA	1.97	0.46
2:B:37:LYS:CE	2:B:130:GLN:HE22	2.29	0.46
2:B:50:TRP:CD2	2:B:111:LEU:HD21	2.51	0.45
2:B:109:ILE:HD11	2:B:121:LYS:CD	2.45	0.45
1:A:115:LYS:NZ	1:A:118:GLU:OE1	2.49	0.45
1:A:137:GLN:NE2	4:A:275:HOH:O	2.47	0.44
2:B:203:LYS:NZ	4:B:380:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ILE:HD11	2:B:172:LEU:HD12	2.01	0.43
2:B:218:ASN:ND2	4:B:334:HOH:O	2.51	0.43
1:A:115:LYS:O	1:A:119:GLU:HG3	2.19	0.42
1:A:88:GLU:CB	1:A:89:PRO:HD3	2.50	0.42
1:A:36:ILE:HD13	1:A:156:LEU:HD21	2.01	0.41
2:B:71:ARG:HB3	2:B:105:ILE:HD11	2.00	0.41
2:B:105:ILE:HG13	2:B:106:PRO:CD	2.41	0.41
2:B:37:LYS:HE2	2:B:130:GLN:HE22	1.86	0.40
2:B:215:LYS:HB2	2:B:222:TYR:CD1	2.57	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	167/191 (87%)	160 (96%)	5 (3%)	2 (1%)	10	7
2	B	185/236 (78%)	177 (96%)	8 (4%)	0	100	100
All	All	352/427 (82%)	337 (96%)	13 (4%)	2 (1%)	21	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ASP
1	A	186	GLU

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	148/176 (84%)	132 (89%)	16 (11%)	6	4
2	B	171/214 (80%)	159 (93%)	12 (7%)	14	11
All	All	319/390 (82%)	291 (91%)	28 (9%)	9	7

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	23	LEU
1	A	38	LYS
1	A	39	GLU
1	A	43	SER
1	A	47	ASN
1	A	75	LEU
1	A	87	LEU
1	A	91	GLN
1	A	94	ARG
1	A	115	LYS
1	A	117	LEU
1	A	124	LEU
1	A	138	ILE
1	A	156	LEU
1	A	191	PHE
2	B	42	GLU
2	B	71	ARG
2	B	72	ASN
2	B	105	ILE
2	B	144	VAL
2	B	149	ILE
2	B	185	LYS
2	B	214	SER
2	B	217	ARG
2	B	228	VAL
2	B	235	GLN
2	B	236	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	91	GLN
1	A	122	GLN
2	B	92	ASN
2	B	130	GLN
2	B	218	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	SO4	B	237	-	4,4,4	0.71	0	6,6,6	0.70	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.