



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:22 AM UTC

PDB ID : 1AOL / pdb_00001aol
Title : FRIEND MURINE LEUKEMIA VIRUS RECEPTOR-BINDING DOMAIN
Authors : Fass, D.; Davey, R.A.; Hamson, C.A.; Kim, P.S.; Cunningham, J.M.; Berger, J.M.
Deposited on : 1997-07-08
Resolution : 2.00 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

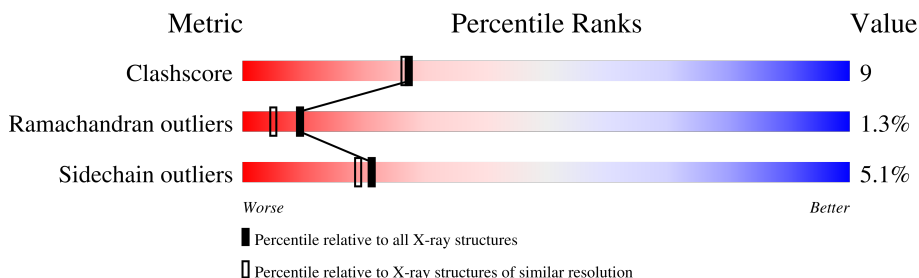
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	228	 70% 23% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2007 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 GP70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1785	1127	313	332	13			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	191	Total 191	O 191	0	0

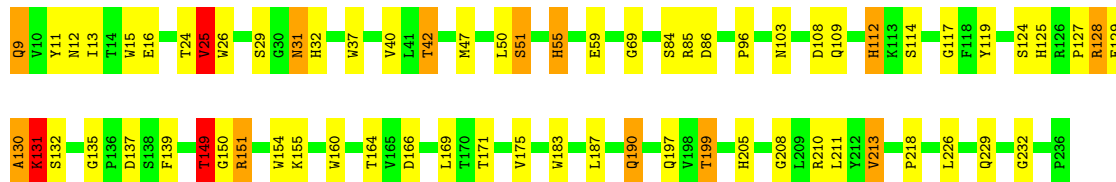
3 Residue-property plots [i](#)

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: GP70

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.30Å 68.40Å 80.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.223 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2007	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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, ZN

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	1.04	7/1849 (0.4%)	1.82	50/2537 (2.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	HIS	CD2-NE2	-7.24	1.29	1.37
1	A	112	HIS	CD2-NE2	-6.98	1.30	1.37
1	A	125	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	205	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	32	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	42	THR	CA-CB	5.09	1.58	1.53
1	A	32	HIS	CG-ND1	-5.09	1.32	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ASN	OD1-CG-ND2	-12.49	110.11	122.60
1	A	25	VAL	CB-CA-C	11.03	121.46	110.65
1	A	12	ASN	CB-CG-ND2	10.92	132.78	116.40
1	A	25	VAL	N-CA-CB	-9.98	98.65	112.12
1	A	85	ARG	CG-CD-NE	-7.66	95.15	112.00
1	A	213	VAL	CB-CA-C	-7.52	97.39	111.30
1	A	199	THR	N-CA-CB	-7.42	99.41	110.61
1	A	25	VAL	N-CA-C	-7.12	106.55	113.53
1	A	205	HIS	CA-CB-CG	-6.43	107.36	113.80
1	A	210	ARG	CB-CG-CD	-6.42	96.53	111.30
1	A	69	GLY	CA-C-N	6.08	124.04	119.66
1	A	69	GLY	C-N-CA	6.08	124.04	119.66
1	A	51	SER	N-CA-CB	-6.04	103.12	112.30
1	A	166	ASP	CA-CB-CG	6.02	118.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	A	160	TRP	CG-CD2-CE3	5.89	139.79	133.90
1	A	130	ALA	CB-CA-C	-5.87	101.05	110.79
1	A	55	HIS	CB-CG-CD2	-5.82	123.63	131.20
1	A	229	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	A	183	TRP	CG-CD2-CE3	5.76	139.66	133.90
1	A	199	THR	O-C-N	-5.72	115.32	122.24
1	A	124	SER	N-CA-C	5.68	119.73	112.34
1	A	9	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	A	149	THR	CB-CA-C	-5.57	100.64	112.78
1	A	205	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	A	213	VAL	N-CA-CB	5.54	120.44	111.36
1	A	86	ASP	CA-CB-CG	-5.53	107.07	112.60
1	A	199	THR	CB-CA-C	5.48	119.43	110.17
1	A	86	ASP	N-CA-C	5.46	117.99	111.71
1	A	31	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	183	TRP	CB-CG-CD1	-5.37	118.84	126.90
1	A	15	TRP	CE2-CD2-CG	-5.36	100.77	107.20
1	A	160	TRP	CE2-CD2-CG	-5.33	100.80	107.20
1	A	85	ARG	NE-CZ-NH2	-5.32	114.41	119.20
1	A	112	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	A	135	GLY	CA-C-N	5.27	125.08	119.28
1	A	135	GLY	C-N-CA	5.27	125.08	119.28
1	A	59	GLU	O-C-N	5.27	128.15	122.15
1	A	232	GLY	CA-C-N	5.24	124.90	119.56
1	A	232	GLY	C-N-CA	5.24	124.90	119.56
1	A	190	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	A	59	GLU	N-CA-C	5.20	117.02	111.36
1	A	109	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	A	103	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	A	137	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	154	TRP	CG-CD2-CE3	5.07	138.97	133.90
1	A	183	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	A	154	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	A	84	SER	CA-C-O	5.03	125.91	120.43
1	A	37	TRP	CG-CD1-NE1	-5.01	103.68	110.20

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	1785	0	1663	32	0
2	A	28	0	26	0	0
3	A	3	0	0	0	0
4	A	191	0	0	4	0
All	All	2007	0	1689	32	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 (32) 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:A:149:THR:HG21	1:A:164:THR:HA	1.47	0.97
1:A:130:ALA:HB2	4:A:289:HOH:O	1.86	0.74
1:A:26:TRP:HB2	1:A:47:MET:HE1	1.67	0.74
1:A:47:MET:SD	4:A:404:HOH:O	2.50	0.69
1:A:26:TRP:HB2	1:A:47:MET:CE	2.24	0.67
1:A:149:THR:HG21	1:A:164:THR:CA	2.24	0.65
1:A:13:ILE:HG23	1:A:226:LEU:HD11	1.83	0.60
1:A:117:GLY:HA3	1:A:151:ARG:HH11	1.69	0.57
1:A:171:THR:HG21	4:A:322:HOH:O	2.06	0.54
1:A:112:HIS:HE1	1:A:169:LEU:O	1.90	0.54
1:A:40:VAL:HG22	1:A:190:GLN:HG2	1.91	0.52
1:A:119:TYR:HA	1:A:150:GLY:HA3	1.91	0.52
1:A:211:LEU:HD12	1:A:218:PRO:HG2	1.94	0.49
1:A:25:VAL:HG13	1:A:47:MET:HB3	1.95	0.47
1:A:47:MET:HE2	1:A:47:MET:HB2	1.76	0.46
1:A:108:ASP:OD2	1:A:171:THR:HG22	2.16	0.46
1:A:117:GLY:HA3	1:A:151:ARG:NH1	2.31	0.46
1:A:108:ASP:O	1:A:112:HIS:HD2	1.98	0.45
1:A:171:THR:O	1:A:175:VAL:HG23	2.17	0.44
1:A:128:ARG:O	1:A:131:LYS:HG3	2.17	0.44
1:A:11:TYR:O	1:A:31:ASN:HA	2.19	0.43
1:A:149:THR:CG2	1:A:164:THR:HA	2.32	0.43
1:A:16:GLU:HB3	1:A:24:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PRO:HA	4:A:393:HOH:O	2.19	0.43
1:A:55:HIS:NE2	1:A:96:PRO:O	2.53	0.42
1:A:42:THR:HA	1:A:187:LEU:O	2.20	0.41
1:A:139:PHE:O	1:A:208:GLY:HA3	2.20	0.41
1:A:26:TRP:CB	1:A:47:MET:HE1	2.45	0.41
1:A:112:HIS:CE1	1:A:169:LEU:O	2.72	0.41
1:A:13:ILE:O	1:A:29:SER:HA	2.20	0.40
1:A:50:LEU:O	1:A:51:SER:HB3	2.21	0.40
1:A:129:GLU:HA	1:A:131:LYS:HE3	2.04	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	226/228 (99%)	217 (96%)	6 (3%)	3 (1%)	9 5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ARG
1	A	131	LYS
1	A	127	PRO

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	197/197 (100%)	187 (95%)	10 (5%)	21	19

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	25	VAL
1	A	114	SER
1	A	131	LYS
1	A	132	SER
1	A	149	THR
1	A	151	ARG
1	A	155	LYS
1	A	199	THR
1	A	213	VAL

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

Mol	Chain	Res	Type
1	A	31	ASN
1	A	112	HIS
1	A	185	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](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	NAG	A	237	1	14,14,15	0.55	0	17,19,21	0.68	0
2	NAG	A	238	1	14,14,15	1.32	2 (14%)	17,19,21	0.81	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
2	NAG	A	237	1	-	1/6/23/26	0/1/1/1
2	NAG	A	238	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	238	NAG	C1-C2	3.04	1.56	1.52
2	A	238	NAG	O5-C5	2.52	1.48	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	237	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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 [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.