



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:30 PM UTC

PDB ID : 1DOT / pdb_00001dot
Title : CRYSTALLOGRAPHIC STRUCTURE OF DUCK OVOTRANSFERRIN AT
2.3 ANGSTROMS RESOLUTION
Authors : Rawas, A.; Muirhead, H.
Deposited on : 1995-08-03
Resolution : 2.35 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

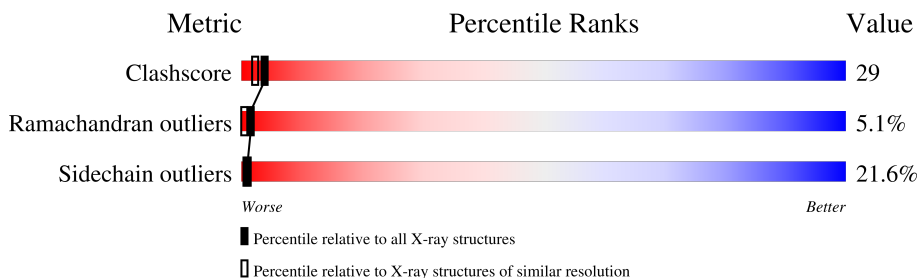
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

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	686	<div> <div style="width: 26%; background-color: green;"></div> <div style="width: 38%; background-color: yellow;"></div> <div style="width: 26%; background-color: orange;"></div> <div style="width: 10%; background-color: red;"></div> </div> <div>26% 38% 26% 10%</div>

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
2	NAG	A	691	-	-	X	-
2	NAG	A	692	-	-	X	-
5	CO3	A	689	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5665 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 DUCK OVOTRANSFERRIN.

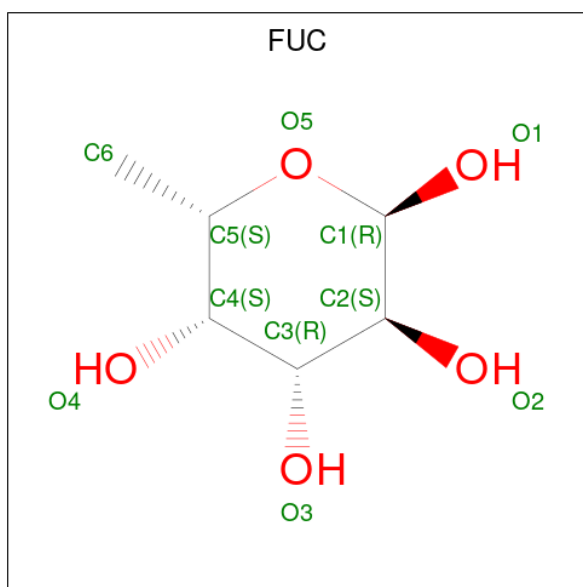
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	686	5299	3325	903	1032	39	0	0	0

- 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
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

- Molecule 3 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).

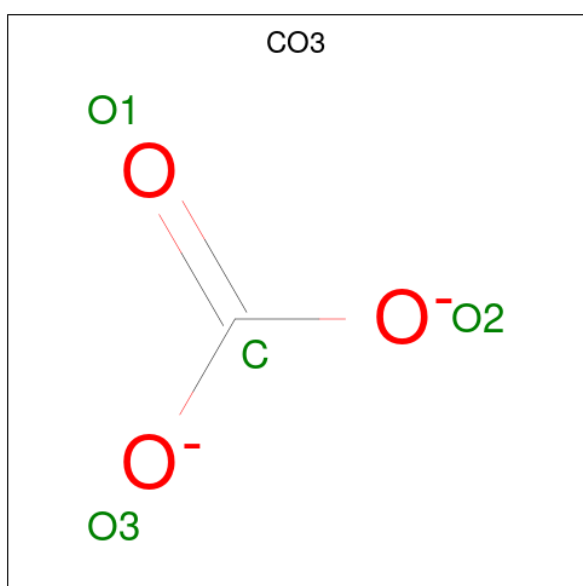


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		

- Molecule 5 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		
5	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is water.

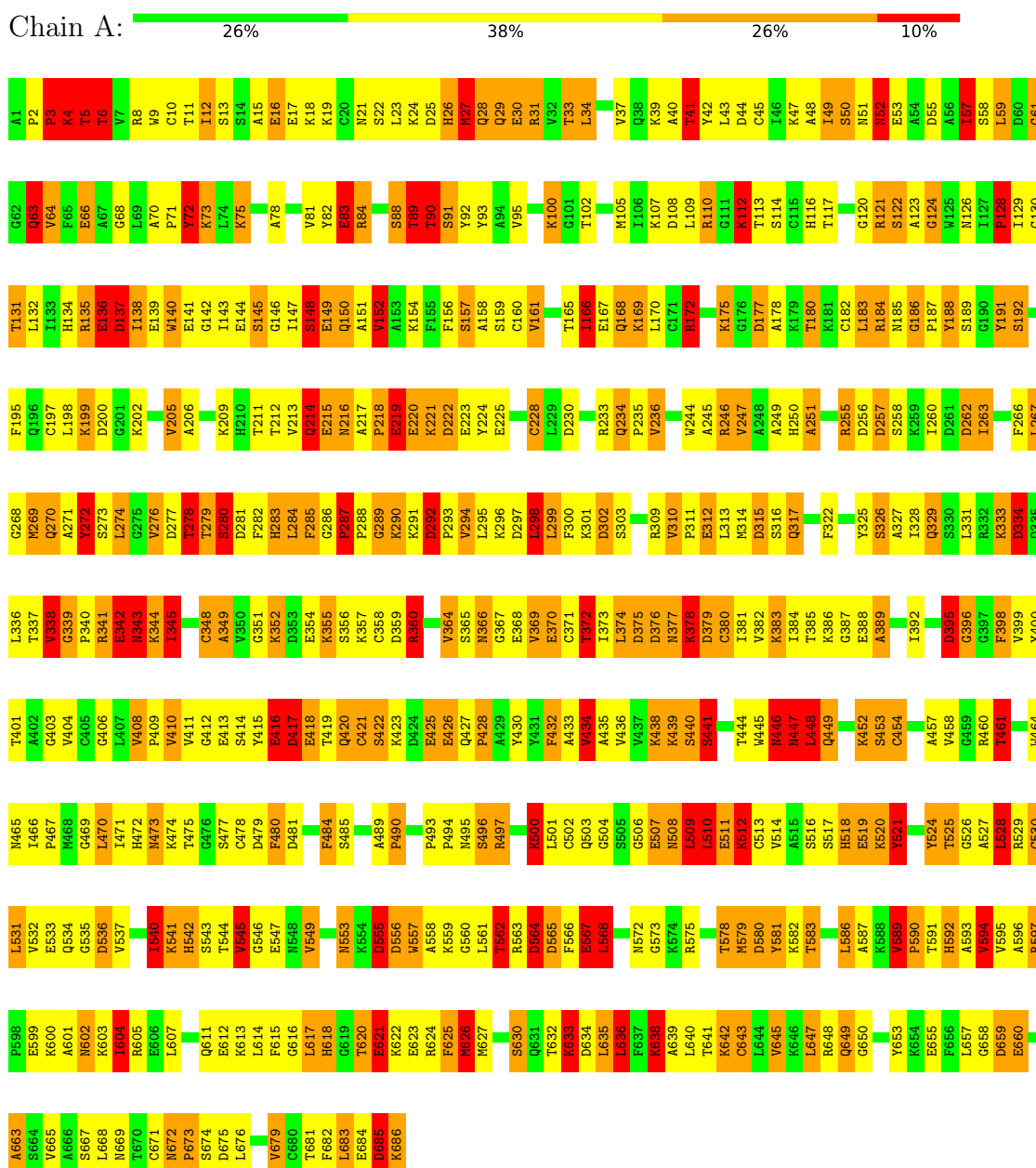
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	318	Total	O	0	0
			318	318		

3 Residue-property plots

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: DUCK OVOTRANSFERRIN



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	49.60Å 85.60Å 178.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.35	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.35)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.230 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5665	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: FE, FUC, CO3, 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	1.69	60/5402 (1.1%)	3.20	707/7292 (9.7%)

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	10

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	ILE	N-CA	-20.34	1.21	1.46
1	A	70	ALA	CA-C	-18.36	1.34	1.53
1	A	136	GLU	N-CA	17.57	1.68	1.46
1	A	82	TYR	C-O	12.99	1.37	1.24
1	A	337	THR	CA-CB	11.12	1.68	1.53

The worst 5 of 707 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	LYS	CA-C-N	27.04	157.99	123.10
1	A	344	LYS	C-N-CA	27.04	157.99	123.10
1	A	417	ASP	CA-C-N	26.06	171.32	121.54
1	A	417	ASP	C-N-CA	26.06	171.32	121.54
1	A	135	ARG	CD-NE-CZ	25.52	160.12	124.40

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	SER	Mainchain
1	A	152	VAL	Mainchain
1	A	27	MET	Mainchain
1	A	3	PRO	Peptide
1	A	5	THR	Peptide

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	5299	0	5186	295	0
2	A	28	0	25	18	0
3	A	10	0	9	3	0
4	A	2	0	0	0	0
5	A	8	0	0	2	0
6	A	318	0	0	27	0
All	All	5665	0	5220	301	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 29.

The worst 5 of 301 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:322:PHE:CB	1:A:597:ARG:HH22	1.23	1.51
1:A:136:GLU:N	1:A:136:GLU:CA	1.68	1.50
1:A:322:PHE:CB	1:A:597:ARG:NH2	1.85	1.40
2:A:692:NAG:C4	3:A:693:FUC:O3	1.72	1.21
1:A:192:SER:HB2	6:A:966:HOH:O	1.41	1.20

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	684/686 (100%)	567 (83%)	82 (12%)	35 (5%)	1 0

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	145	SER
1	A	177	ASP
1	A	280	SER
1	A	287	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	578/578 (100%)	453 (78%)	125 (22%)	1 1

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	PRO
1	A	604	ILE
1	A	375	ASP
1	A	602	ASN
1	A	638	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	473	ASN
1	A	669	ASN
1	A	553	ASN
1	A	329	GLN
1	A	472	HIS

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
5	CO3	A	689	4	3,3,3	1.74	1 (33%)	2,3,3	0.75	0
2	NAG	A	692	-	14,14,15	1.44	3 (21%)	17,19,21	1.94	4 (23%)
2	NAG	A	691	-	14,14,15	1.59	4 (28%)	17,19,21	1.86	6 (35%)
3	FUC	A	693	-	10,10,11	0.89	0	14,14,16	2.13	6 (42%)
5	CO3	A	690	4	3,3,3	1.82	1 (33%)	2,3,3	1.53	1 (50%)

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	691	-	-	3/6/23/26	0/1/1/1
2	NAG	A	692	-	-	1/6/23/26	0/1/1/1
3	FUC	A	693	-	-	-	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	691	NAG	O7-C7	-3.65	1.15	1.23
2	A	692	NAG	O7-C7	-3.33	1.15	1.23
5	A	690	CO3	O1-C	3.13	1.36	1.25
5	A	689	CO3	O1-C	2.98	1.36	1.25
2	A	691	NAG	C3-C2	-2.55	1.47	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	692	NAG	C3-C4-C5	4.59	118.55	110.23
3	A	693	FUC	O3-C3-C2	4.34	118.92	110.05
2	A	692	NAG	O5-C1-C2	-3.97	105.15	111.29
3	A	693	FUC	O3-C3-C4	3.67	119.04	110.38
2	A	691	NAG	C1-O5-C5	3.23	116.52	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	691	NAG	C4-C5-C6-O6
2	A	691	NAG	O5-C5-C6-O6
2	A	692	NAG	O5-C5-C6-O6
2	A	691	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	689	CO3	2	0
2	A	692	NAG	7	0
2	A	691	NAG	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	693	FUC	3	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.