



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1WSZ  
Title : Mutant human ABO(H) blood group transferase A  
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Deposited on : 2004-11-12  
Resolution : 1.59 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

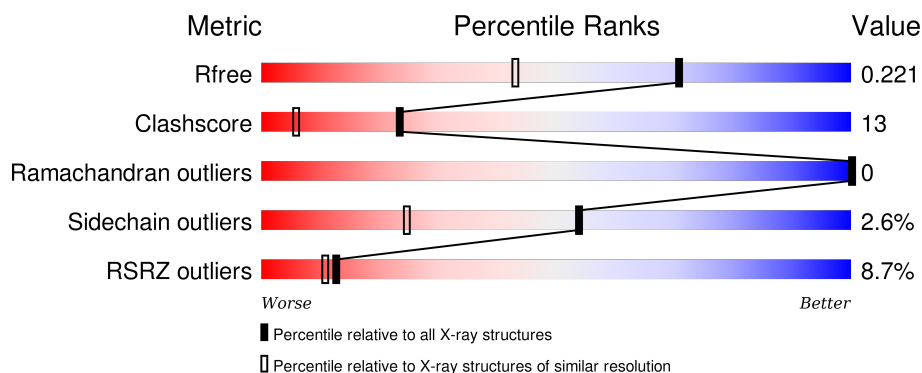
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.59 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))
$R_{free}$	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	292	<div> <div>8%</div> <div>71%</div> <div>17%</div> <div>• 10%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2365 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 Histo-blood group ABO system transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2145	1394	366	375	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	INITIATING METHIONINE	UNP P16442
A	74	SER	PRO	ENGINEERED MUTATION	UNP P16442

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

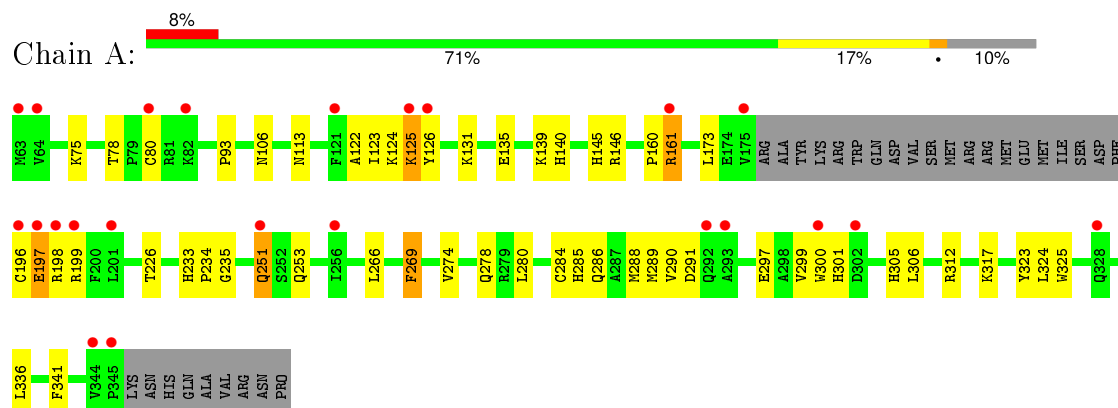
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Hg	0	0
			4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	216	Total	O	0	0
			216	216		



- Molecule 1: Histo-blood group ABO system transferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.70 Å   150.10 Å   79.70 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 1.59 19.86 – 1.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.59) 98.6 (19.86-1.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 1.59 Å)	Xtriage
Refinement program	unknown	Depositor
R, $R_{free}$	0.209   ,   0.244 0.201   ,   0.221	Depositor DCC
$R_{free}$ test set	261 reflections (10.73%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 42619 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2365	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0/2205	0.61	0/2997

There are no bond length outliers.

There are no bond angle outliers.

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	2145	0	2130	57	0
2	A	4	0	0	0	0
3	A	216	0	0	2	0
All	All	2365	0	2130	57	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 13.

All (57) 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:125:LYS:HD3	1:A:125:LYS:H	1.24	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ARG:HA	1:A:161:ARG:NE	1.82	0.93
1:A:123:ILE:HG22	1:A:124:LYS:HG3	1.57	0.84
1:A:233:HIS:HD2	1:A:235:GLY:H	1.24	0.83
1:A:266:LEU:HD13	1:A:324:LEU:HD13	1.65	0.77
1:A:125:LYS:HD3	1:A:125:LYS:N	1.99	0.75
1:A:139:LYS:HD3	1:A:139:LYS:O	1.86	0.74
1:A:226:THR:HG21	1:A:317:LYS:HB2	1.69	0.74
1:A:251:GLN:H	1:A:251:GLN:NE2	1.86	0.73
1:A:196:CYS:HA	1:A:198:ARG:NH1	2.06	0.71
1:A:196:CYS:HB2	1:A:199:ARG:NH2	2.06	0.71
1:A:125:LYS:H	1:A:125:LYS:CD	2.03	0.69
1:A:199:ARG:HB3	1:A:199:ARG:NH1	2.12	0.64
1:A:233:HIS:CD2	1:A:235:GLY:H	2.13	0.64
1:A:285:HIS:O	1:A:289:MET:HG3	1.98	0.64
1:A:139:LYS:HD2	1:A:140:HIS:NE2	2.14	0.63
1:A:274:VAL:O	1:A:278:GLN:HG3	2.00	0.61
1:A:251:GLN:HE21	1:A:251:GLN:H	1.49	0.60
1:A:75:LYS:HB2	1:A:78:THR:HB	1.84	0.59
1:A:233:HIS:HA	1:A:266:LEU:HG	1.83	0.59
1:A:325:TRP:CZ3	1:A:336:LEU:HD11	2.38	0.59
1:A:139:LYS:HD2	1:A:140:HIS:CE1	2.39	0.58
1:A:123:ILE:CG2	1:A:124:LYS:HG3	2.32	0.57
1:A:93:PRO:HG2	1:A:317:LYS:HG2	1.89	0.55
1:A:284:CYS:O	1:A:288:MET:HG3	2.07	0.54
1:A:113:ASN:HD21	1:A:146:ARG:HH11	1.55	0.54
1:A:269:PHE:HB2	1:A:324:LEU:HD12	1.91	0.53
1:A:196:CYS:HA	1:A:198:ARG:HH12	1.73	0.53
1:A:323:TYR:O	1:A:341:PHE:HB3	2.08	0.53
1:A:234:PRO:HD3	1:A:266:LEU:HD11	1.92	0.51
1:A:122:ALA:C	1:A:123:ILE:HD12	2.33	0.49
1:A:106:ASN:OD1	1:A:145:HIS:HE1	1.96	0.48
1:A:125:LYS:HE2	1:A:126:TYR:CE1	2.49	0.48
1:A:139:LYS:HD3	1:A:139:LYS:C	2.34	0.48
1:A:280:LEU:HD23	1:A:280:LEU:C	2.33	0.48
1:A:197:GLU:CD	1:A:197:GLU:H	2.17	0.47
1:A:197:GLU:HB3	1:A:278:GLN:NE2	2.29	0.47
1:A:305:HIS:HE1	3:A:552:HOH:O	1.97	0.47
1:A:286:GLN:O	1:A:290:VAL:HG23	2.15	0.47
1:A:113:ASN:ND2	1:A:146:ARG:HH11	2.13	0.47
1:A:160:PRO:HG3	3:A:712:HOH:O	2.15	0.46
1:A:199:ARG:HH11	1:A:199:ARG:HB3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ARG:HA	1:A:161:ARG:HE	1.76	0.46
1:A:197:GLU:OE1	1:A:197:GLU:N	2.49	0.45
1:A:325:TRP:CE3	1:A:336:LEU:HD11	2.52	0.44
1:A:325:TRP:CH2	1:A:336:LEU:HD11	2.52	0.44
1:A:251:GLN:N	1:A:251:GLN:NE2	2.61	0.44
1:A:123:ILE:HD12	1:A:123:ILE:N	2.33	0.43
1:A:299:VAL:HG13	1:A:300:TRP:N	2.34	0.43
1:A:131:LYS:O	1:A:135:GLU:HG3	2.18	0.43
1:A:312:ARG:HD3	1:A:312:ARG:HA	1.74	0.42
1:A:288:MET:HG2	1:A:305:HIS:CE1	2.53	0.42
1:A:113:ASN:HD21	1:A:146:ARG:NH1	2.17	0.42
1:A:173:LEU:HD22	1:A:173:LEU:N	2.34	0.42
1:A:306:LEU:HD23	1:A:306:LEU:C	2.41	0.41
1:A:297:GLU:OE2	1:A:301:HIS:HD2	2.03	0.41
1:A:253:GLN:HG2	1:A:291:ASP:OD1	2.21	0.40

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	259/292 (89%)	252 (97%)	7 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	233/260 (90%)	227 (97%)	6 (3%)	54 25

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	CYS
1	A	125	LYS
1	A	161	ARG
1	A	197	GLU
1	A	251	GLN
1	A	269	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	145	HIS
1	A	155	GLN
1	A	233	HIS
1	A	251	GLN
1	A	278	GLN
1	A	286	GLN
1	A	301	HIS
1	A	305	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	263/292 (90%)	0.52	23 (8%) 13 11	15, 24, 39, 56	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	CYS	10.8
1	A	80	CYS	9.9
1	A	345	PRO	6.7
1	A	63	MET	5.8
1	A	197	GLU	5.3
1	A	64	VAL	5.3
1	A	82	LYS	5.0
1	A	161	ARG	4.9
1	A	175	VAL	3.4
1	A	201	LEU	3.2
1	A	121	PHE	3.1
1	A	251	GLN	3.0
1	A	256	ILE	3.0
1	A	199	ARG	2.7
1	A	344	VAL	2.6
1	A	125	LYS	2.6
1	A	292	GLN	2.6
1	A	126	TYR	2.3
1	A	198	ARG	2.3
1	A	293	ALA	2.3
1	A	300	TRP	2.3
1	A	328	GLN	2.2
1	A	302	ASP	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HG	A	404	1/1	0.99	0.06	-1.94	41,41,41,41	1
2	HG	A	401	1/1	0.98	0.05	-	43,43,43,43	1
2	HG	A	403	1/1	0.99	0.05	-	40,40,40,40	0
2	HG	A	402	1/1	0.99	0.05	-	47,47,47,47	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.