



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:38 PM BST

PDB ID : 1SUV  
Title : Structure of Human Transferrin Receptor-Transferrin Complex  
Authors : Cheng, Y.; Zak, O.; Aisen, P.; Harrison, S.C.; Walz, T.  
Deposited on : 2004-03-26  
Resolution : 7.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

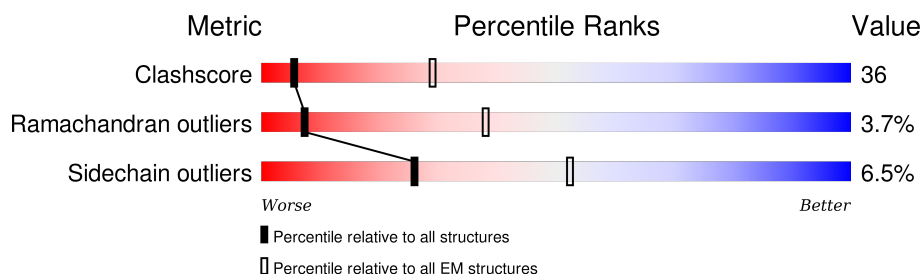
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.50 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	639	
1	B	639	
2	C	329	
2	D	329	
3	E	345	
3	F	345	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20612 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	639	Total	C	N	O	S	0	0
			5056	3244	846	952	14		
1	B	639	Total	C	N	O	S	0	0
			5056	3244	846	952	14		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	GLU	GLN	SEE REMARK 999	UNP P02786
A	613	GLU	ARG	SEE REMARK 999	UNP P02786
B	172	GLU	GLN	SEE REMARK 999	UNP P02786
B	613	GLU	ARG	SEE REMARK 999	UNP P02786

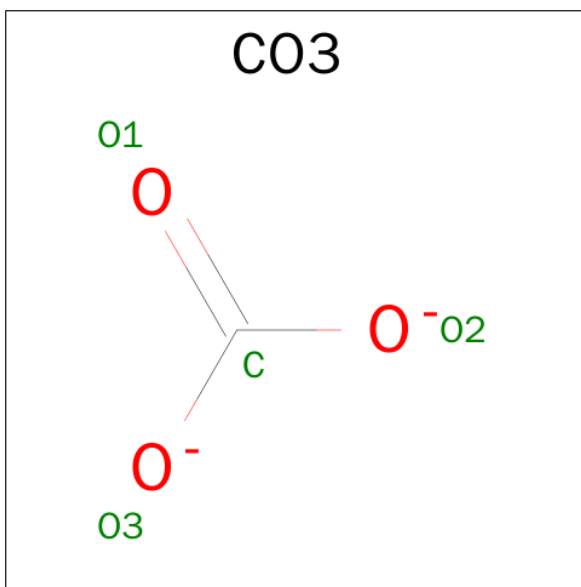
- Molecule 2 is a protein called Serotransferrin, N-lobe.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	329	Total	C	N	O	S	5	0
			2567	1621	440	485	21		
2	D	329	Total	C	N	O	S	5	0
			2567	1621	440	485	21		

- Molecule 3 is a protein called Serotransferrin, C-lobe.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	345	Total	C	N	O	S	0	0
			2669	1662	469	512	26		
3	F	345	Total	C	N	O	S	0	0
			2669	1662	469	512	26		

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
4	C	1	Total	C	O	1
			8	2	6	
4	D	1	Total	C	O	1
			8	2	6	
4	E	1	Total	C	O	0
			4	1	3	
4	F	1	Total	C	O	0
			4	1	3	

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Fe	0
			1	1	
5	C	1	Total	Fe	0
			1	1	
5	F	1	Total	Fe	0
			1	1	
5	E	1	Total	Fe	0
			1	1	

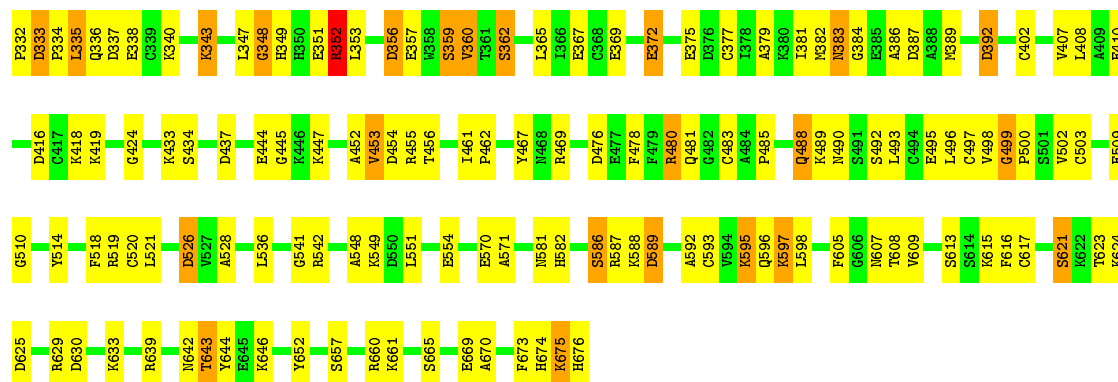






• Molecule 3: Serotransferrin, C-lobe

Chain F: 60% 33% 7%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction for each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 FILM	Depositor



## 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: CO3, FE

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.38	0/5177	0.61	1/7021 (0.0%)
1	B	0.38	0/5177	0.61	1/7021 (0.0%)
2	C	0.84	0/2648	0.88	5/3578 (0.1%)
2	D	0.84	0/2648	0.88	5/3578 (0.1%)
3	E	0.89	0/2723	1.03	9/3675 (0.2%)
3	F	0.89	0/2723	1.03	9/3675 (0.2%)
All	All	0.67	0/21096	0.81	30/28548 (0.1%)

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	88	LYS	N-CA-CB	12.30	132.73	110.60
2	D	88	LYS	N-CA-CB	12.28	132.70	110.60
3	F	437	ASP	CB-CG-OD2	11.00	128.20	118.30
3	E	437	ASP	CB-CG-OD2	10.97	128.17	118.30
2	C	88	LYS	CA-CB-CG	-10.21	90.94	113.40

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	5056	0	4980	582	0
1	B	5056	0	4982	575	0
2	C	2567	0	2482	94	0
2	D	2567	0	2482	95	0
3	E	2669	0	2574	197	0
3	F	2669	0	2575	205	0
4	C	8	0	0	0	0
4	D	8	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	20612	0	20075	1446	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 36.

The worst 5 of 1446 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:D:317:TYR:CE1	3:F:383:ASN:HB2	1.19	1.66
2:C:317:TYR:CE1	3:E:383:ASN:HB2	1.19	1.65
1:B:623:ARG:HD2	3:F:360:VAL:CG2	1.16	1.62
1:A:623:ARG:CD	3:E:360:VAL:HG23	1.14	1.59
1:A:623:ARG:HB3	3:E:360:VAL:CG2	1.34	1.56

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 PDB entries followed by that with respect to all EM entries.

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	637/639 (100%)	499 (78%)	100 (16%)	38 (6%)	2	26
1	B	637/639 (100%)	497 (78%)	101 (16%)	39 (6%)	2	26
2	C	332/329 (101%)	315 (95%)	15 (4%)	2 (1%)	30	74
2	D	332/329 (101%)	315 (95%)	15 (4%)	2 (1%)	30	74
3	E	343/345 (99%)	309 (90%)	26 (8%)	8 (2%)	8	48
3	F	343/345 (99%)	309 (90%)	26 (8%)	8 (2%)	8	48
All	All	2624/2626 (100%)	2244 (86%)	283 (11%)	97 (4%)	7	37

5 of 97 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	210	VAL
1	A	251	ASN
1	A	330	PRO
1	A	361	SER

### 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 PDB entries followed by that with respect to all EM entries.

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	548/548 (100%)	505 (92%)	43 (8%)	16	51
1	B	548/548 (100%)	507 (92%)	41 (8%)	17	53
2	C	279/274 (102%)	275 (99%)	4 (1%)	74	89
2	D	279/274 (102%)	275 (99%)	4 (1%)	74	89
3	E	292/293 (100%)	266 (91%)	26 (9%)	12	44
3	F	292/293 (100%)	266 (91%)	26 (9%)	12	44
All	All	2238/2230 (100%)	2094 (94%)	144 (6%)	26	58

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	457	ASP

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Mol	Chain	Res	Type
1	B	732	ARG
3	F	586	SER
1	B	537	LEU
1	B	606	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	164	ASN
1	B	335	GLN
2	D	152	ASN
1	B	191	GLN
1	B	275	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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
4	CO3	C	338[A]	5	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	C	338[B]	5	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	D	338[A]	5	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	D	338[B]	5	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	E	701	5	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	F	701	5	0,3,3	0.00	-	0,3,3	0.00	-

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	CO3	C	338[A]	5	-	0/0/0/0	0/0/0/0
4	CO3	C	338[B]	5	-	0/0/0/0	0/0/0/0
4	CO3	D	338[A]	5	-	0/0/0/0	0/0/0/0
4	CO3	D	338[B]	5	-	0/0/0/0	0/0/0/0
4	CO3	E	701	5	-	0/0/0/0	0/0/0/0
4	CO3	F	701	5	-	0/0/0/0	0/0/0/0

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.