



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3SN2 / pdb_00003sn2
Title : Crystal structure analysis of iron regulatory protein 1 in complex with transferrin receptor IRE B RNA
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Deposited on : 2011-06-28
Resolution : 2.99 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

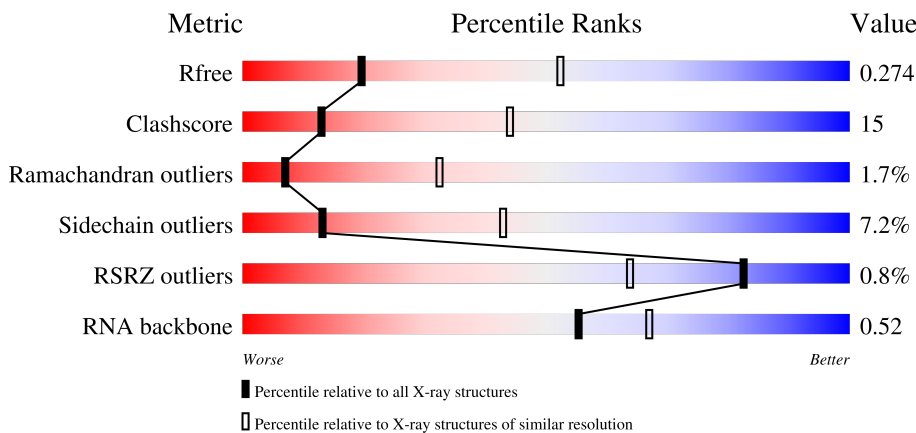
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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 $\leq 5\%$. 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	908	59% 31% 7%
2	B	29	62% 34%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14323 atoms, of which 6934 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 Cytoplasmic aconitate hydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	848	Total	C	H	N	O	S	0	0	0
			13259	4241	6627	1138	1229	24			

There are 24 discrepancies between the modelled and reference sequences:

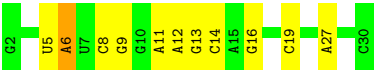
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP Q01059
A	-17	GLY	-	expression tag	UNP Q01059
A	-16	HIS	-	expression tag	UNP Q01059
A	-15	HIS	-	expression tag	UNP Q01059
A	-14	HIS	-	expression tag	UNP Q01059
A	-13	HIS	-	expression tag	UNP Q01059
A	-12	HIS	-	expression tag	UNP Q01059
A	-11	HIS	-	expression tag	UNP Q01059
A	-10	ALA	-	expression tag	UNP Q01059
A	-9	ASP	-	expression tag	UNP Q01059
A	-8	ASP	-	expression tag	UNP Q01059
A	-7	ASP	-	expression tag	UNP Q01059
A	-6	ASP	-	expression tag	UNP Q01059
A	-5	LYS	-	expression tag	UNP Q01059
A	-4	ASP	-	expression tag	UNP Q01059
A	-3	GLY	-	expression tag	UNP Q01059
A	-2	VAL	-	expression tag	UNP Q01059
A	-1	ASP	-	expression tag	UNP Q01059
A	0	LYS	-	expression tag	UNP Q01059
A	1	LEU	-	expression tag	UNP Q01059
A	283	PRO	LEU	SEE REMARK 999	UNP Q01059
A	437	SER	CYS	engineered mutation	UNP Q01059
A	503	SER	CYS	engineered mutation	UNP Q01059
A	874	PHE	LEU	SEE REMARK 999	UNP Q01059

- Molecule 2 is a RNA chain called transferrin receptor iron regulatory element B RNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	29	Total 918	C 275	H 307	N 107	O 201	P 28	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total 131	O 131	0	0
3	B	15	Total 15	O 15	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.67Å 101.67Å 281.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.64 – 2.99 32.64 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (32.64-2.99) 99.7 (32.64-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.227 , 0.275 0.226 , 0.274	Depositor DCC
R_{free} test set	2000 reflections (6.51%)	wwPDB-VP
Wilson B-factor (Å ²)	99.5	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 98.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14323	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.36	0/6785	0.78	4/9210 (0.0%)
2	B	0.17	0/682	0.36	0/1060
All	All	0.35	0/7467	0.75	4/10270 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	513	LEU	CA-C-N	6.73	126.76	119.90
1	A	513	LEU	C-N-CA	6.73	126.76	119.90
1	A	464	LYS	CA-C-N	6.36	126.57	119.32
1	A	464	LYS	C-N-CA	6.36	126.57	119.32

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	6632	6627	6643	209	0
2	B	611	307	313	4	0
3	A	131	0	0	1	0
3	B	15	0	0	0	0
All	All	7389	6934	6956	213	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 15.

The worst 5 of 213 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:188:VAL:HG21	1:A:320:LEU:HD11	1.69	0.72
1:A:396:LYS:HA	1:A:403:GLN:HB3	1.71	0.72
1:A:605:ILE:HB	1:A:606:PRO:HD3	1.72	0.70
1:A:744:LEU:HB2	1:A:745:PRO:HD3	1.73	0.70
1:A:252:HIS:ND1	1:A:253:PRO:HD2	2.07	0.69

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	840/908 (92%)	733 (87%)	93 (11%)	14 (2%)	7	32

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	648	PHE
1	A	403	GLN
1	A	578	ASN
1	A	746	SER

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	723/772 (94%)	671 (93%)	52 (7%)	13	43

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	464	LYS
1	A	577	THR
1	A	813	VAL
1	A	484	GLU
1	A	513	LEU

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	726	ASN
1	A	804	HIS
1	A	743	HIS
1	A	409	HIS
1	A	679	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	28/29 (96%)	6 (21%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	6	A
2	B	8	C
2	B	9	G
2	B	16	G
2	B	19	C

There are no RNA pucker outliers to report.

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](#)

There are no ligands in this entry.

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](#)

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, 95th 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 ²)	Q<0.9
1	A	848/908 (93%)	-0.06	7 (0%) 82 64	80, 130, 173, 187	0
2	B	29/29 (100%)	-0.47	0 100 100	104, 123, 142, 145	0
All	All	877/937 (93%)	-0.07	7 (0%) 82 64	80, 129, 173, 187	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	4.3
1	A	147	PHE	3.0
1	A	688	ARG	2.6
1	A	512	PRO	2.4
1	A	149	ARG	2.4

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.