W O R L D W I D E

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P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 26, 2014 – 09:49 PM GMT

PDB ID : 2RB8
Title : High resolution design of a protein loop
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Deposited on : 2007-09-18
Resolution : 1.45 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 1.45 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	Percentile Ranks	Value
Clashscore		15
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		9.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution
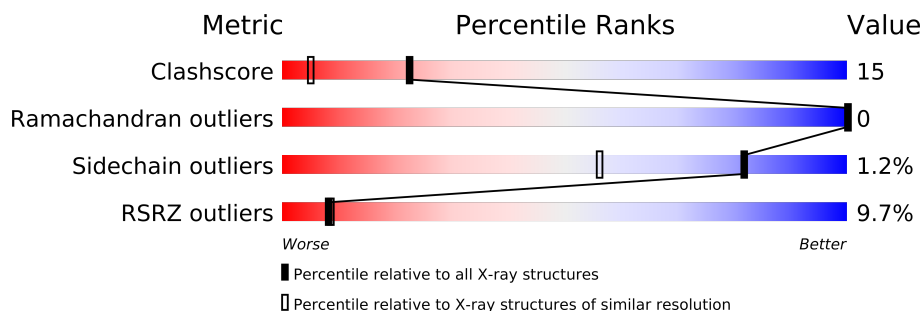
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2834 (1.50-1.42)
Ramachandran outliers	78287	2769 (1.50-1.42)
Sidechain outliers	78261	2767 (1.50-1.42)
RSRZ outliers	66119	2477 (1.50-1.42)

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 >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	104	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 801 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Tenascin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	93	723	449	116	155	3	0	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	801	MET	-	INITIATING METHIONINE	UNP P24821
A	824	MET	PHE	ENGINEERED	UNP P24821
A	825	PRO	LYS	ENGINEERED	UNP P24821
A	827	SER	LEU	ENGINEERED	UNP P24821
A	828	GLN	ALA	ENGINEERED	UNP P24821
A	829	PRO	GLU	ENGINEERED	UNP P24821
A	830	VAL	ILE	ENGINEERED	UNP P24821
A	833	PHE	ILE	ENGINEERED	UNP P24821
A	894	ALA	-	EXPRESSION TAG	UNP P24821
A	895	ALA	-	EXPRESSION TAG	UNP P24821
A	896	ALA	-	EXPRESSION TAG	UNP P24821
A	897	LEU	-	EXPRESSION TAG	UNP P24821
A	898	GLU	-	EXPRESSION TAG	UNP P24821
A	899	HIS	-	EXPRESSION TAG	UNP P24821
A	900	HIS	-	EXPRESSION TAG	UNP P24821
A	901	HIS	-	EXPRESSION TAG	UNP P24821
A	902	HIS	-	EXPRESSION TAG	UNP P24821
A	903	HIS	-	EXPRESSION TAG	UNP P24821
A	904	HIS	-	EXPRESSION TAG	UNP P24821

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	78	78	78	0	0

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

• Molecule 1: Tenascin

Chain A:
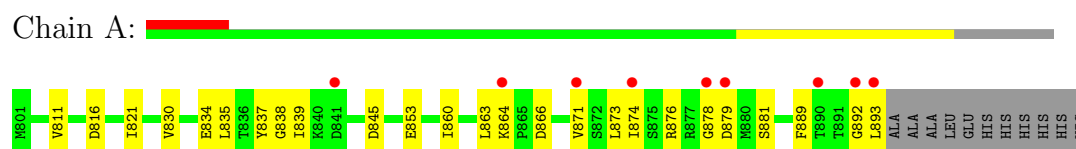
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	62.78Å 62.78Å 53.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.45 27.18 – 1.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.45) 90.0 (27.18-1.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 1.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.170 , 0.196 0.300 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 39.1	EDS
Estimated twinning fraction	0.423 for -h,-k,l	Xtriage
L-test for twinning	$< |L| > = 0.39, < L^2 > = 0.21$	Xtriage
Outliers	0 of 19907 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	801	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0/736	0.63	0/1003

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	723	0	698	21	1
2	A	78	0	0	0	0
All	All	801	0	698	21	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

The worst 5 of 21 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:839:ILE:HD11	1:A:864:LYS:HD3	1.46	0.96
1:A:821:ILE:HD13	1:A:871:VAL:HG11	1.74	0.69
1:A:821:ILE:HD11	1:A:860:ILE:HD12	1.84	0.59
1:A:835:LEU:HD21	1:A:860:ILE:HD11	1.85	0.58
1:A:837:TYR:CG	1:A:860:ILE:HD13	2.41	0.55

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:864:LYS:NZ	1:A:864:LYS:NZ[4_646]	1.85	0.35

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	91/104 (88%)	87 (96%)	4 (4%)	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	84/92 (91%)	83 (99%)	1 (1%)	82	56

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	873	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	862	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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, 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	93/104 (89%)	0.69	9 (9%)	8	8	8, 14, 26, 30	4 (4%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	892	GLY	6.0
1	A	893	LEU	3.3
1	A	878	GLY	3.2
1	A	874	ILE	2.9
1	A	879	ASP	2.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.