

wwPDB X-ray Structure Validation Summary Report (i)

Nov 22, 2023 – 05:00 PM JST

PDB ID	:	7X9G
Title	:	Crystal structure of human EDA and EDAR
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Deposited on		
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

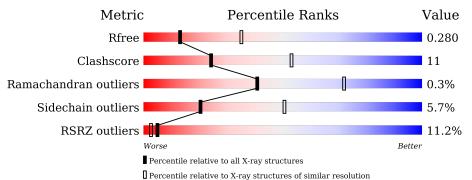
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.80 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	А	159	.% •		79%			9%	·	9%
1	В	159	9%		66%			23%	•	10%
2	С	123	20%	42%		20%	•	35%	_	



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2853 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 Ectodysplasin-A, secreted form.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	144	Total	С	Ν	0	S	0	0	0
	A	144	1124	719	190	209	6	0	0	0
1	В	143	Total	С	Ν	0	S	0	0	0
	D	140	1119	716	189	208	6	0	U	0

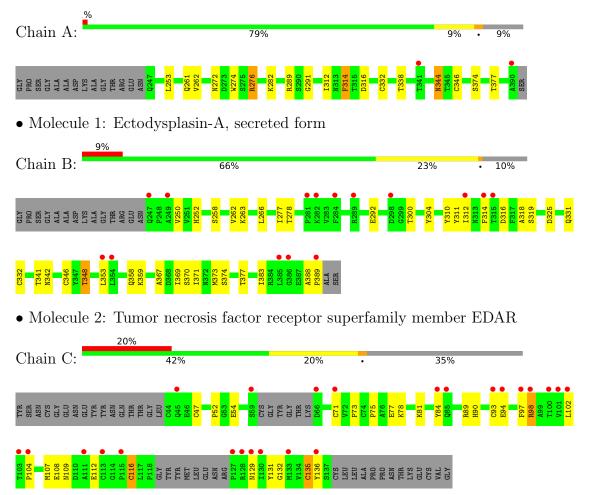
• Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member EDAR.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	С	80	Total 610	C 377	N 101	O 120	S 12	0	0	0



3 Residue-property plots (i)

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 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: Ectodysplasin-A, secreted form



4 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	87.17Å 87.17Å 156.35Å	Denesiten
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.71 - 2.80	Depositor
Resolution (A)	43.58 - 2.80	EDS
% Data completeness	90.9 (34.71-2.80)	Depositor
(in resolution range)	90.9(43.58-2.80)	EDS
R _{merge}	0.04	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.68 (at 2.81 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D D.	0.248 , 0.282	Depositor
R, R_{free}	0.248 , 0.280	DCC
R_{free} test set	407 reflections $(4.11%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	41.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31,48.7	EDS
L-test for twinning ²	$< L > = 0.48, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.058 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	2853	wwPDB-VP
Average B, all atoms $(Å^2)$	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.38	0/1148	0.72	2/1556~(0.1%)	
1	В	0.34	0/1143	0.62	0/1549	
2	С	0.42	0/626	0.67	0/844	
All	All	0.38	0/2917	0.67	2/3949~(0.1%)	

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
2	С	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	261	GLN	N-CA-C	-10.79	81.86	111.00
1	А	262	VAL	N-CA-CB	-7.56	94.88	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	С	98	ARG	Sidechain

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1124	0	1118	10	0
1	В	1119	0	1113	31	0
2	С	610	0	549	29	0
All	All	2853	0	2780	62	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 11.

The worst 5 of 62 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:C:81:LYS:HG2	2:C:108:GLU:HA	1.37	1.02
1:B:292:GLU:OE1	1:B:359:LYS:HD3	1.65	0.96
1:B:325:ASP:CG	1:B:358:GLN:HE22	1.73	0.91
1:B:341:THR:CG2	2:C:94:GLU:HG3	2.03	0.88
1:B:341:THR:HG21	2:C:94:GLU:O	1.79	0.82

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	Perce	ntiles
1	А	142/159~(89%)	131 (92%)	10 (7%)	1 (1%)	22	53
1	В	141/159~(89%)	135~(96%)	6 (4%)	0	100	100
2	С	74/123~(60%)	64 (86%)	10 (14%)	0	100	100
All	All	357/441 (81%)	330 (92%)	26 (7%)	1 (0%)	41	72

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	314	PHE

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	А	123/133~(92%)	117~(95%)	6~(5%)	25 57
1	В	123/133~(92%)	120 (98%)	3 (2%)	49 81
2	С	68/104~(65%)	59~(87%)	9 (13%)	4 12
All	All	314/370~(85%)	296 (94%)	18 (6%)	20 50

5 of 18 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	С	116	CYS
2	С	136	TYR
2	С	135	CYS
1	В	348	THR
2	С	97	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	256	GLN
1	А	344	ASN
1	В	358	GLN
1	В	372	ASN
2	С	90	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 monosaccharides 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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	144/159~(90%)	0.16	2 (1%) 75 70	12, 36, 64, 81	0
1	В	143/159~(89%)	0.62	15 (10%) 6 3	20, 52, 96, 112	0
2	С	80/123~(65%)	1.43	24 (30%) 0 0	39, 67, 113, 122	0
All	All	367/441~(83%)	0.62	41 (11%) 5 3	12, 51, 97, 122	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	389	PRO	5.8
2	С	59	SER	5.7
2	С	128	ARG	5.0
2	С	130	ILE	4.8
2	С	127	PRO	4.4

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 monosaccharides 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.

