



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 28, 2020 – 12:12 PM EDT

PDB ID : 6E8F
Title : Crystal Structure of Human Protocadherin-15 EC3-5 CD2-1
Authors : Choudhary, D.; Tamilselvan, E.; Sotomayor, M.
Deposited on : 2018-07-29
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)	:	2.14.6

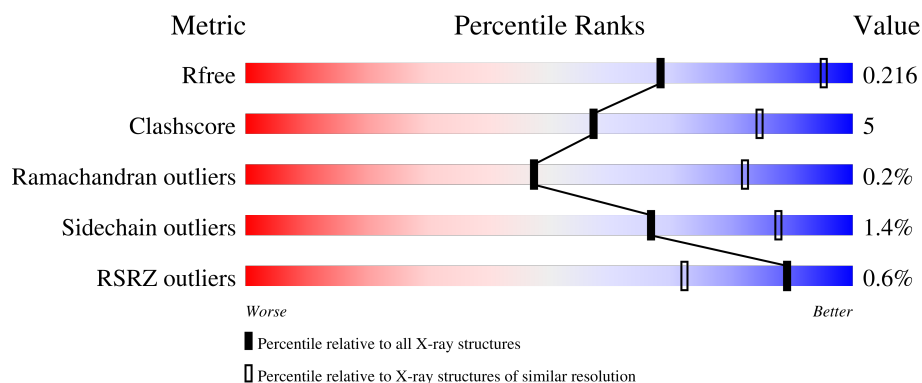
1 Overall quality at a glance

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	362	 83% 11% • 5%
1	B	362	 82% 13% 5%
1	C	362	 80% 12% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7988 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 Protocadherin-15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2678	1710	430	529	9			
1	C	333	Total	C	N	O	S	0	0	0
			2594	1650	424	512	8			
1	B	345	Total	C	N	O	S	0	0	0
			2694	1720	432	533	9			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	-	initiating methionine	UNP Q96QU1
A	595	LEU	-	expression tag	UNP Q96QU1
A	596	GLU	-	expression tag	UNP Q96QU1
A	597	HIS	-	expression tag	UNP Q96QU1
A	598	HIS	-	expression tag	UNP Q96QU1
A	599	HIS	-	expression tag	UNP Q96QU1
A	600	HIS	-	expression tag	UNP Q96QU1
A	601	HIS	-	expression tag	UNP Q96QU1
A	602	HIS	-	expression tag	UNP Q96QU1
C	241	MET	-	initiating methionine	UNP Q96QU1
C	595	LEU	-	expression tag	UNP Q96QU1
C	596	GLU	-	expression tag	UNP Q96QU1
C	597	HIS	-	expression tag	UNP Q96QU1
C	598	HIS	-	expression tag	UNP Q96QU1
C	599	HIS	-	expression tag	UNP Q96QU1
C	600	HIS	-	expression tag	UNP Q96QU1
C	601	HIS	-	expression tag	UNP Q96QU1
C	602	HIS	-	expression tag	UNP Q96QU1
B	241	MET	-	initiating methionine	UNP Q96QU1
B	595	LEU	-	expression tag	UNP Q96QU1
B	596	GLU	-	expression tag	UNP Q96QU1
B	597	HIS	-	expression tag	UNP Q96QU1
B	598	HIS	-	expression tag	UNP Q96QU1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	599	HIS	-	expression tag	UNP Q96QU1
B	600	HIS	-	expression tag	UNP Q96QU1
B	601	HIS	-	expression tag	UNP Q96QU1
B	602	HIS	-	expression tag	UNP Q96QU1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	5	Total Ca 5 5	0	0
2	A	4	Total Ca 4 4	0	0
2	C	4	Total Ca 4 4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0


- Molecule 4 is water.

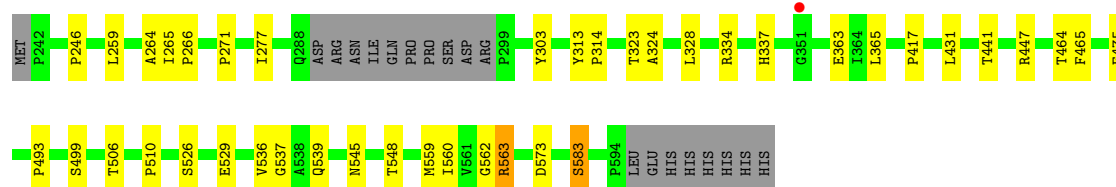
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	C	3	Total O 3 3	0	0
4	B	2	Total O 2 2	0	0

3 Residue-property plots


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.

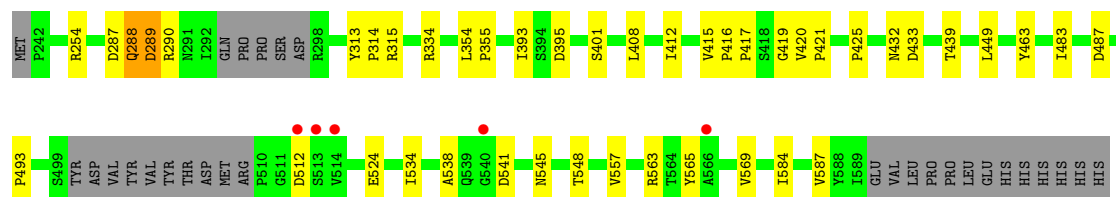
• Molecule 1: Protocadherin-15

Chain A: 




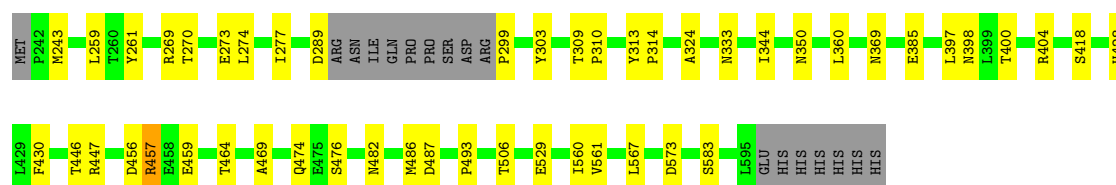
• Molecule 1: Protocadherin-15

Chain C: 



• Molecule 1: Protocadherin-15

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	95.73Å 95.91Å 258.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.95 – 2.99 47.95 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.95-2.99) 98.4 (47.95-2.99)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.174 , 0.214 0.175 , 0.216	Depositor DCC
R_{free} test set	2321 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.199 for k,h,-l	Xtriage
Reported twinning fraction	0.768 for H, K, L 0.232 for -K, -H, -L	Depositor
Outliers	0 of 48290 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7988	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

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

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	0.46	0/2744	0.68	0/3765
1	B	0.44	0/2760	0.67	1/3787 (0.0%)
1	C	0.40	0/2654	0.64	0/3636
All	All	0.44	0/8158	0.67	1/11188 (0.0%)

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
1	A	0	3
1	B	0	3
1	C	0	3
All	All	0	9

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	385	GLU	CB-CA-C	-6.42	97.55	110.40

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	447	ARG	Sidechain
1	A	562	GLY	Peptide
1	A	563	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	254	ARG	Sidechain
1	C	315	ARG	Sidechain

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	2678	0	2623	26	0
1	B	2694	0	2638	27	0
1	C	2594	0	2547	26	0
2	A	4	0	0	0	0
2	B	5	0	0	0	0
2	C	4	0	0	0	0
3	A	1	0	0	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
All	All	7988	0	7808	78	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 5.

The worst 5 of 78 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:B:493:PRO:O	1:B:583:SER:HB3	1.75	0.86
1:B:269:ARG:NH1	1:B:273:GLU:OE2	2.27	0.67
1:B:529:GLU:O	1:B:573:ASP:HA	2.01	0.61
1:C:420:VAL:N	1:C:421:PRO:HD3	2.16	0.60
1:C:395:ASP:OD1	1:C:401:SER:OG	2.18	0.60

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	339/362 (94%)	317 (94%)	21 (6%)	1 (0%)	41	76
1	B	341/362 (94%)	326 (96%)	15 (4%)	0	100	100
1	C	327/362 (90%)	306 (94%)	20 (6%)	1 (0%)	41	76
All	All	1007/1086 (93%)	949 (94%)	56 (6%)	2 (0%)	47	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	417	PRO
1	C	493	PRO

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	305/324 (94%)	300 (98%)	5 (2%)	62	86
1	B	307/324 (95%)	304 (99%)	3 (1%)	76	91
1	C	295/324 (91%)	290 (98%)	5 (2%)	60	85
All	All	907/972 (93%)	894 (99%)	13 (1%)	67	88

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	287	ASP

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Mol	Chain	Res	Type
1	C	288	GLN
1	B	243	MET
1	A	583	SER
1	C	512	ASP

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

Mol	Chain	Res	Type
1	A	368	ASN
1	C	288	GLN
1	C	474	GLN
1	B	474	GLN
1	B	482	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 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 [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	343/362 (94%)	-0.11	1 (0%) 94 84	53, 78, 124, 164	0
1	B	345/362 (95%)	-0.10	0 100 100	49, 77, 128, 168	0
1	C	333/362 (91%)	-0.05	5 (1%) 73 46	55, 104, 149, 173	0
All	All	1021/1086 (94%)	-0.09	6 (0%) 89 72	49, 83, 138, 173	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	514	VAL	3.9
1	C	566	ALA	3.2
1	C	512	ASP	3.0
1	A	351	GLY	2.4
1	C	513	SER	2.2

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](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(\AA^2)	Q<0.9
3	NA	A	705	1/1	0.94	0.07	75,75,75,75	0
2	CA	B	703	1/1	0.96	0.17	95,95,95,95	0
2	CA	B	705	1/1	0.97	0.13	103,103,103,103	0
2	CA	B	701	1/1	0.97	0.24	69,69,69,69	0
2	CA	A	703	1/1	0.98	0.24	77,77,77,77	0
2	CA	C	702	1/1	0.98	0.17	107,107,107,107	0
2	CA	C	704	1/1	0.98	0.15	116,116,116,116	0
2	CA	C	701	1/1	0.99	0.14	89,89,89,89	0
2	CA	B	702	1/1	0.99	0.21	68,68,68,68	0
2	CA	A	704	1/1	0.99	0.19	64,64,64,64	0
2	CA	A	702	1/1	1.00	0.18	58,58,58,58	0
2	CA	A	701	1/1	1.00	0.17	76,76,76,76	0
2	CA	B	704	1/1	1.00	0.18	70,70,70,70	0
2	CA	C	703	1/1	1.00	0.12	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.