



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:24 PM UTC

PDB ID : 6I8G / pdb_00006i8g
Title : Structure of the plant immune signaling node EDS1 (enhanced disease susceptibility 1) in complex with nanobody ENB73
Authors : Niefind, K.; Voss, M.; Toelzer, C.
Deposited on : 2018-11-20
Resolution : 2.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

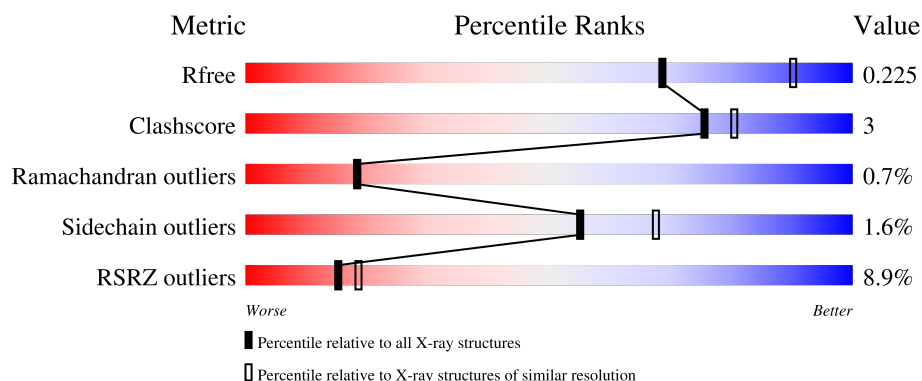
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	631	10% 88% 10% ..
2	B	143	% 82% 6% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6170 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 Protein EDS1L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	618	Total	C	N	O	S	0	2	0
			5029	3192	871	947	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	624	LEU	-	expression tag	UNP Q9XF23
A	625	GLU	-	expression tag	UNP Q9XF23
A	626	HIS	-	expression tag	UNP Q9XF23
A	627	HIS	-	expression tag	UNP Q9XF23
A	628	HIS	-	expression tag	UNP Q9XF23
A	629	HIS	-	expression tag	UNP Q9XF23
A	630	HIS	-	expression tag	UNP Q9XF23
A	631	HIS	-	expression tag	UNP Q9XF23

- Molecule 2 is a protein called EDS1-specific nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			972	607	170	191	4			

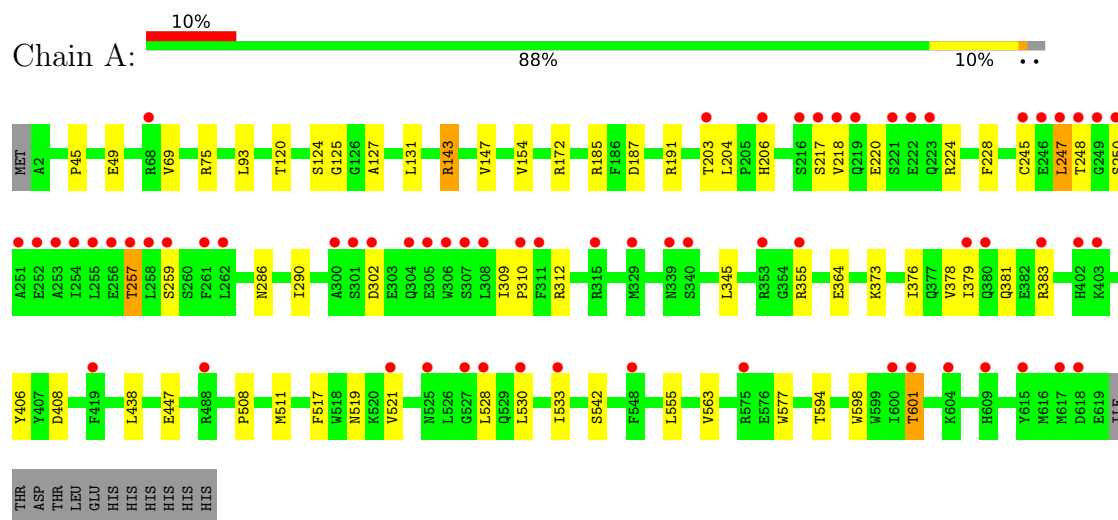
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total	O	0	0
			123	123		
3	B	46	Total	O	0	0
			46	46		

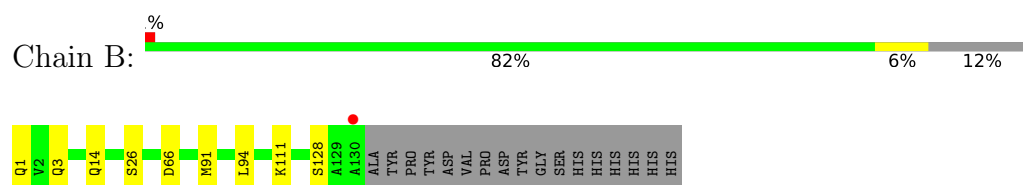
3 Residue-property plots [i](#)

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: Protein EDS1L



• Molecule 2: EDS1-specific nanobody



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.50Å 68.23Å 105.27Å 90.00° 123.44° 90.00°	Depositor
Resolution (Å)	52.57 – 2.34 52.57 – 2.34	Depositor EDS
% Data completeness (in resolution range)	71.1 (52.57-2.34) 71.1 (52.57-2.34)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.194 , 0.222 0.196 , 0.225	Depositor DCC
R_{free} test set	1295 reflections (2.92%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6170	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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

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	0.13	0/5142	0.32	0/6944
2	B	0.12	0/993	0.35	0/1350
All	All	0.13	0/6135	0.33	0/8294

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5029	0	4934	33	0
2	B	972	0	931	4	0
3	A	123	0	0	1	0
3	B	46	0	0	0	0
All	All	6170	0	5865	36	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 3.

All (36) 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:B:91:MET:HE2	2:B:94:LEU:HD21	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:HH22	1:A:302:ASP:HB3	1.61	0.65
1:A:49:GLU:HG3	1:A:204:LEU:HD23	1.82	0.61
1:A:93:LEU:HD22	1:A:131:LEU:HB3	1.83	0.59
1:A:245:CYS:O	1:A:250:SER:N	2.29	0.57
1:A:373:LYS:O	1:A:376:ILE:HG13	2.04	0.57
2:B:1:GLN:N	2:B:1:GLN:OE1	2.36	0.55
1:A:247:LEU:HD21	1:A:364:GLU:HG3	1.90	0.53
1:A:511:MET:HE1	1:A:519:ASN:ND2	2.24	0.52
1:A:309:ILE:HG23	1:A:310:PRO:HD3	1.91	0.51
1:A:257:THR:C	1:A:259:SER:H	2.20	0.50
1:A:528:LEU:HB2	1:A:533:ILE:HD11	1.93	0.49
1:A:408:ASP:OD1	1:A:594:THR:OG1	2.23	0.49
1:A:598:TRP:O	1:A:601:THR:HG22	2.13	0.49
1:A:45:PRO:HB3	1:A:125:GLY:H	1.78	0.48
1:A:124:SER:O	1:A:127:ALA:HB3	2.13	0.48
1:A:187:ASP:O	1:A:191:ARG:NH1	2.43	0.48
1:A:206[A]:HIS:CD2	1:A:224:ARG:HH21	2.32	0.48
1:A:185:ARG:HH12	1:A:302:ASP:HB3	1.80	0.47
1:A:120:THR:HA	1:A:154:VAL:O	2.15	0.46
1:A:75:ARG:NH1	3:A:707:HOH:O	2.49	0.46
1:A:530:LEU:H	1:A:530:LEU:HD12	1.80	0.46
1:A:286:ASN:O	1:A:290:ILE:HG13	2.17	0.45
1:A:172:ARG:HA	1:A:447:GLU:HA	1.99	0.44
1:A:143:ARG:HD2	1:A:508:PRO:O	2.17	0.44
1:A:376:ILE:HA	1:A:379:ILE:HG12	2.00	0.44
1:A:555:LEU:HD22	1:A:563:VAL:HB	2.00	0.43
1:A:438:LEU:HD23	1:A:438:LEU:HA	1.90	0.43
1:A:217:SER:OG	2:B:111:LYS:NZ	2.51	0.43
1:A:542:SER:HA	1:A:577:TRP:HH2	1.83	0.43
1:A:378:VAL:O	1:A:381:GLN:HG2	2.19	0.42
1:A:511:MET:HE2	1:A:511:MET:HB3	1.90	0.42
1:A:345:LEU:HD12	1:A:355[B]:ARG:HG2	2.02	0.42
1:A:203:THR:HG23	1:A:228:PHE:HD1	1.86	0.41
2:B:3:GLN:HB2	2:B:26:SER:HB3	2.02	0.41
1:A:517:PHE:O	1:A:521:VAL:HG13	2.20	0.41

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	618/631 (98%)	590 (96%)	24 (4%)	4 (1%)	21	22
2	B	124/143 (87%)	120 (97%)	3 (2%)	1 (1%)	16	16
All	All	742/774 (96%)	710 (96%)	27 (4%)	5 (1%)	18	18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	128	SER
1	A	220	GLU
1	A	248	THR
1	A	257	THR
1	A	218	VAL

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	545/556 (98%)	537 (98%)	8 (2%)	57	69
2	B	102/117 (87%)	100 (98%)	2 (2%)	48	61
All	All	647/673 (96%)	637 (98%)	10 (2%)	55	69

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	143	ARG
1	A	147	VAL
1	A	247	LEU
1	A	312	ARG
1	A	383	ARG
1	A	406	TYR
1	A	601	THR
2	B	14	GLN
2	B	66	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	292	GLN
1	A	529	GLN
2	B	5	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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	618/631 (97%)	0.46	65 (10%) 11 13	23, 51, 115, 222	2 (0%)
2	B	126/143 (88%)	-0.14	1 (0%) 82 85	32, 43, 65, 88	0
All	All	744/774 (96%)	0.36	66 (8%) 15 18	23, 48, 107, 222	2 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	LEU	5.8
1	A	254	ILE	5.8
1	A	253	ALA	5.4
1	A	251	ALA	5.0
1	A	255	LEU	5.0
1	A	218	VAL	5.0
1	A	302	ASP	4.7
1	A	615	TYR	4.3
1	A	618	ASP	4.3
1	A	301	SER	4.2
1	A	203	THR	4.0
1	A	306	TRP	4.0
1	A	311	PHE	3.9
1	A	248	THR	3.5
1	A	259	SER	3.5
1	A	530	LEU	3.4
1	A	247	LEU	3.4
1	A	604	LYS	3.3
1	A	217	SER	3.2
1	A	257	THR	3.1
1	A	528	LEU	3.0
1	A	355[A]	ARG	3.0
1	A	216	SER	3.0
1	A	403	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	310	PRO	2.9
2	B	130	ALA	2.9
1	A	68	ARG	2.8
1	A	250	SER	2.8
1	A	307	SER	2.8
1	A	308	LEU	2.8
1	A	304	GLN	2.7
1	A	300	ALA	2.7
1	A	206[A]	HIS	2.7
1	A	419	PHE	2.6
1	A	339	ASN	2.6
1	A	221	SER	2.6
1	A	380	GLN	2.5
1	A	256	GLU	2.4
1	A	527	GLY	2.4
1	A	600	ILE	2.4
1	A	261	PHE	2.4
1	A	340	SER	2.3
1	A	533	ILE	2.3
1	A	249	GLY	2.3
1	A	329	MET	2.3
1	A	601	THR	2.3
1	A	353	ARG	2.3
1	A	521	VAL	2.2
1	A	525	ASN	2.2
1	A	617	MET	2.2
1	A	245	CYS	2.2
1	A	315	ARG	2.2
1	A	383	ARG	2.2
1	A	252	GLU	2.2
1	A	219	GLN	2.1
1	A	402	HIS	2.1
1	A	548	PHE	2.1
1	A	222	GLU	2.1
1	A	305	GLU	2.0
1	A	223	GLN	2.0
1	A	379	ILE	2.0
1	A	488	ARG	2.0
1	A	246	GLU	2.0
1	A	609	HIS	2.0
1	A	262	LEU	2.0
1	A	575	ARG	2.0

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.