Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 10:43 pm GMT

PDB ID	:	2XQH
Title	:	Crystal structure of an immunoglobulin-binding fragment of the trimeric autotransporter adhesin EibD
Authors	:	Leo, J.C.; Lyskowski, A.; Hartmann, M.; Schwarz, H.; Linke, D.; Lupas, A.N.; Goldman, A.
Deposited on	:	2010-09-02
Resolution	:	1.99 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:

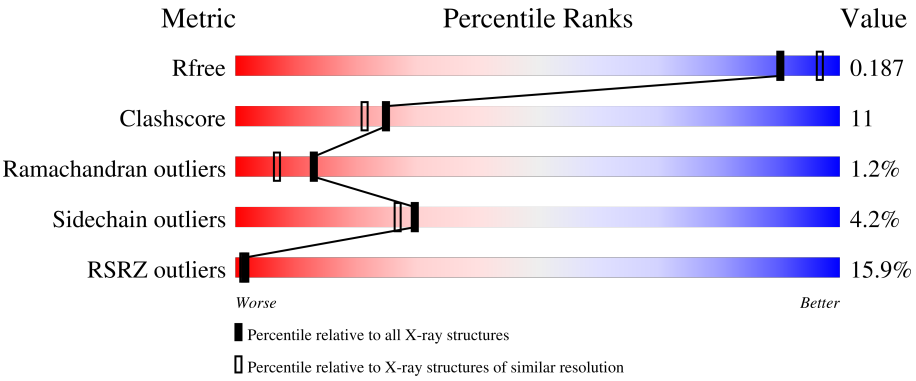
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	A	281	15% 75% 14% · 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2039 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 IMMUNOGLOBULIN-BINDING PROTEIN EIBD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	0	0	0
			1862	1122	341	399			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MET	-	expression tag	UNP Q9MCI8
A	139	GLY	-	expression tag	UNP Q9MCI8
A	140	SER	-	expression tag	UNP Q9MCI8
A	141	SER	-	expression tag	UNP Q9MCI8
A	142	HIS	-	expression tag	UNP Q9MCI8
A	143	HIS	-	expression tag	UNP Q9MCI8
A	144	HIS	-	expression tag	UNP Q9MCI8
A	145	HIS	-	expression tag	UNP Q9MCI8
A	146	HIS	-	expression tag	UNP Q9MCI8
A	147	HIS	-	expression tag	UNP Q9MCI8
A	148	SER	-	expression tag	UNP Q9MCI8
A	149	SER	-	expression tag	UNP Q9MCI8
A	150	GLY	-	expression tag	UNP Q9MCI8
A	151	LEU	-	expression tag	UNP Q9MCI8
A	152	VAL	-	expression tag	UNP Q9MCI8
A	153	PRO	-	expression tag	UNP Q9MCI8
A	154	ARG	-	expression tag	UNP Q9MCI8
A	155	GLY	-	expression tag	UNP Q9MCI8
A	156	SER	-	expression tag	UNP Q9MCI8
A	157	HIS	-	expression tag	UNP Q9MCI8
A	158	MET	-	expression tag	UNP Q9MCI8
A	159	ALA	-	expression tag	UNP Q9MCI8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Cl 4 4	0	0

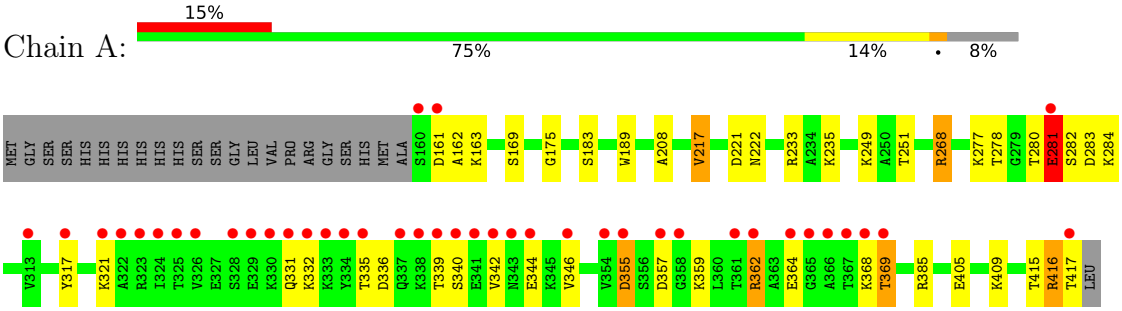
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	173	Total O 173 173	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: IMMUNOGLOBULIN-BINDING PROTEIN EIBD



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	48.95Å 48.95Å 409.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.51 – 1.99 42.17 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.8 (41.51-1.99) 97.9 (42.17-1.99)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.97 (at 2.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.159 , 0.185 0.157 , 0.187	Depositor DCC
R_{free} test set	1232 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.074 for -h-k,k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2039	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL

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	0.41	0/1874	0.56	0/2534

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	1862	0	1844	40	0
2	A	4	0	0	0	0
3	A	173	0	0	8	1
All	All	2039	0	1844	40	1

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.

All (40) 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:268:ARG:HH11	1:A:268:ARG:HG3	1.21	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASP:HB3	1:A:162:ALA:HA	1.52	0.92
1:A:417:THR:HA	3:A:2170:HOH:O	1.74	0.87
1:A:161:ASP:CB	1:A:162:ALA:HA	2.13	0.79
1:A:161:ASP:HB3	1:A:162:ALA:CA	2.15	0.77
1:A:280:THR:O	1:A:281:GLU:HB3	1.84	0.77
1:A:268:ARG:HG3	1:A:268:ARG:NH1	1.95	0.75
1:A:415:THR:O	1:A:416:ARG:HB2	1.84	0.75
1:A:268:ARG:HH11	1:A:268:ARG:CG	2.05	0.68
1:A:342:VAL:O	1:A:346:VAL:HG23	2.03	0.58
1:A:277:LYS:HD2	3:A:2061:HOH:O	2.03	0.58
1:A:417:THR:HG21	3:A:2168:HOH:O	2.03	0.58
1:A:161:ASP:CB	1:A:162:ALA:CA	2.80	0.57
1:A:362:ARG:HB3	1:A:364:GLU:HG3	1.87	0.56
1:A:317:TYR:CE2	1:A:321:LYS:HE2	2.40	0.56
1:A:416:ARG:O	1:A:417:THR:C	2.43	0.55
1:A:278:THR:HG21	1:A:284:LYS:O	2.06	0.55
1:A:233:ARG:HD3	3:A:2045:HOH:O	2.08	0.53
1:A:331:GLN:O	1:A:335:THR:HG23	2.08	0.53
1:A:161:ASP:HB3	1:A:162:ALA:C	2.30	0.52
1:A:280:THR:O	1:A:280:THR:HG22	2.12	0.49
1:A:340:SER:O	1:A:344:GLU:HG2	2.13	0.48
1:A:161:ASP:HB3	1:A:163:LYS:N	2.29	0.47
1:A:175:GLY:HA3	1:A:189:TRP:CE3	2.50	0.47
1:A:409:LYS:NZ	3:A:2166:HOH:O	2.48	0.47
1:A:233:ARG:NH2	1:A:249:LYS:HD3	2.31	0.46
1:A:282:SER:HB3	1:A:284:LYS:CG	2.46	0.46
1:A:208:ALA:HB2	1:A:221:ASP:O	2.16	0.46
1:A:217:VAL:HG12	1:A:217:VAL:O	2.15	0.46
1:A:405:GLU:OE1	3:A:2163:HOH:O	2.20	0.46
1:A:385:ARG:NE	3:A:2140:HOH:O	2.18	0.46
1:A:284:LYS:H	1:A:284:LYS:HG2	1.47	0.45
1:A:355:ASP:HB2	1:A:359:LYS:O	2.17	0.45
1:A:235:LYS:HE3	1:A:251:THR:HG23	2.00	0.44
1:A:368:LYS:HG3	1:A:369:THR:N	2.32	0.43
1:A:169:SER:HA	1:A:183:SER:O	2.19	0.43
1:A:336:ASP:O	1:A:339:THR:HG22	2.18	0.42
1:A:416:ARG:HD3	1:A:416:ARG:HA	1.73	0.42
1:A:282:SER:HB3	1:A:284:LYS:HG2	2.02	0.41
1:A:283:ASP:OD2	3:A:2096:HOH:O	2.22	0.40

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	Interatomic distance (Å)	Clash overlap (Å)
3:A:2071:HOH:O	3:A:2167:HOH:O[9_554]	2.13	0.07

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	256/281 (91%)	250 (98%)	3 (1%)	3 (1%)	13 7

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	GLU
1	A	416	ARG
1	A	217	VAL

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	190/209 (91%)	182 (96%)	8 (4%)	30 27

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	A	268	ARG
1	A	281	GLU

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Mol	Chain	Res	Type
1	A	332	LYS
1	A	355	ASP
1	A	357	ASP
1	A	362	ARG
1	A	369	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	ASN
1	A	407	ASN
1	A	414	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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

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, 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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	258/281 (91%)	0.70	41 (15%) 1 1	17, 32, 93, 122	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	326	VAL	5.6
1	A	342	VAL	5.3
1	A	337	GLN	4.9
1	A	324	ILE	4.4
1	A	334	TYR	4.2
1	A	367	THR	4.2
1	A	417	THR	4.1
1	A	161	ASP	4.1
1	A	333	LYS	4.0
1	A	328	SER	3.9
1	A	344	GLU	3.9
1	A	339	THR	3.8
1	A	335	THR	3.7
1	A	354	VAL	3.7
1	A	317	TYR	3.6
1	A	331	GLN	3.6
1	A	366	ALA	3.6
1	A	364	GLU	3.5
1	A	332	LYS	3.4
1	A	369	THR	3.4
1	A	338	LYS	3.4
1	A	361	THR	3.4
1	A	358	GLY	3.2
1	A	341	GLU	3.2
1	A	330	LYS	3.2
1	A	368	LYS	3.1
1	A	357	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	321	LYS	2.8
1	A	322	ALA	2.5
1	A	340	SER	2.5
1	A	362	ARG	2.5
1	A	365	GLY	2.4
1	A	329	GLU	2.4
1	A	346	VAL	2.4
1	A	323	ARG	2.3
1	A	325	THR	2.2
1	A	281	GLU	2.2
1	A	160	SER	2.1
1	A	313	VAL	2.1
1	A	343	ASN	2.0
1	A	355	ASP	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 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, 95^{th} 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(Å^2)	Q<0.9
2	CL	A	1421	1/1	0.97	0.09	58,58,58,58	1
2	CL	A	1419	1/1	0.99	0.09	29,29,29,29	1
2	CL	A	1420	1/1	0.99	0.14	23,23,23,23	1
2	CL	A	1418	1/1	0.99	0.07	39,39,39,39	1

6.5 Other polymers (i)

There are no such residues in this entry.