



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7DAA
Title : Crystal structure of basigin complexed with anti-basigin Fab fragment
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Deposited on : 2020-10-16
Resolution : 2.51 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

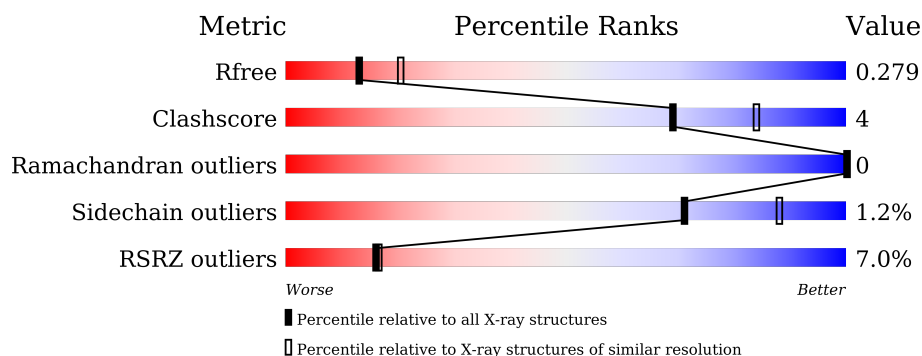
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	176	<div> <div>15%</div> <div>39% 10% 51%</div> </div>
2	L	218	<div> <div>90% 9%</div> </div>
3	H	217	<div> <div>4%</div> <div>88% 9% .</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3885 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 Isoform 2 of Basigin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	86	Total	C	N	O	S	0	0	0
			675	419	122	130	4			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	-	expression tag	UNP P35613
A	152	GLN	ASN	engineered mutation	UNP P35613
A	186	GLN	ASN	engineered mutation	UNP P35613
A	270	ASP	-	expression tag	UNP P35613
A	271	TYR	-	expression tag	UNP P35613
A	272	LYS	-	expression tag	UNP P35613
A	273	ASP	-	expression tag	UNP P35613
A	274	ASP	-	expression tag	UNP P35613
A	275	ASP	-	expression tag	UNP P35613
A	276	ASP	-	expression tag	UNP P35613
A	277	LYS	-	expression tag	UNP P35613

- Molecule 2 is a protein called Light chain of antibody Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	217	Total	C	N	O	S	0	0	0
			1630	1022	267	334	7			

- Molecule 3 is a protein called Heavy chain of antibody Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	212	Total	C	N	O	S	0	0	0
			1564	994	251	314	5			

- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Cd 2	0	0
4	L	10	Total 10	Cd 10	0	0
4	H	4	Total 4	Cd 4	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.34Å 247.35Å 52.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.68 – 2.51 123.68 – 2.51	Depositor EDS
% Data completeness (in resolution range)	68.4 (123.68-2.51) 68.5 (123.68-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.19rc2_4022	Depositor
R, R_{free}	0.228 , 0.283 0.228 , 0.279	Depositor DCC
R_{free} test set	948 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3885	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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: PCA, CD

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	0.25	0/688	0.53	0/927
2	L	0.27	0/1663	0.50	0/2264
3	H	0.26	0/1597	0.49	0/2187
All	All	0.26	0/3948	0.50	0/5378

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	675	0	662	9	0
2	L	1630	0	1578	10	0
3	H	1564	0	1536	9	0
4	A	2	0	0	0	0
4	H	4	0	0	0	0
4	L	10	0	0	0	0
All	All	3885	0	3776	28	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 4.

All (28) 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:L:7:GLN:HE21	2:L:22:ILE:HD11	1.48	0.77
1:A:124:LEU:HD12	1:A:169:LEU:HD23	1.74	0.69
2:L:38:GLN:HB2	2:L:48:LEU:HD11	1.79	0.64
1:A:122:ALA:HB2	1:A:174:LEU:HD11	1.82	0.62
3:H:126:SER:H	3:H:129:SER:HB3	1.65	0.62
2:L:9:PRO:O	2:L:106:THR:OG1	2.10	0.59
2:L:191:GLU:OE1	2:L:215:ARG:NH1	2.38	0.56
2:L:95:ILE:HD13	2:L:100:ALA:HB2	1.86	0.56
1:A:194:ASP:OD1	1:A:195:GLN:N	2.40	0.54
3:H:118:PRO:HB3	3:H:144:TYR:HB3	1.88	0.54
3:H:129:SER:OG	3:H:136:ALA:O	2.27	0.52
2:L:124:PRO:HD3	2:L:136:VAL:HG22	1.92	0.51
1:A:136:ASP:HB2	1:A:188:THR:HB	1.93	0.51
2:L:3:VAL:HG23	2:L:98:TYR:HB3	1.94	0.50
3:H:121:PHE:HD2	3:H:140:LEU:HD23	1.76	0.50
1:A:107:VAL:HG13	1:A:194:ASP:HB3	1.94	0.49
1:A:179:ASP:N	1:A:180:PRO:HD2	2.28	0.48
2:L:34:LEU:HD13	2:L:72:PHE:CG	2.50	0.47
3:H:3:VAL:HG12	3:H:23:VAL:HG12	1.96	0.47
3:H:65:ARG:NH2	3:H:86:ASP:OD1	2.48	0.47
1:A:186:GLN:HG3	1:A:195:GLN:HE21	1.81	0.46
2:L:144:TYR:CG	2:L:145:PRO:HA	2.52	0.45
1:A:116:ILE:O	1:A:202:VAL:HA	2.17	0.44
3:H:167:ALA:HB2	3:H:177:LEU:HD23	1.99	0.43
2:L:111:LYS:HA	2:L:144:TYR:OH	2.19	0.42
3:H:142:LYS:NZ	3:H:170:GLN:HE22	2.17	0.41
3:H:33:MET:HG3	3:H:75:VAL:HG21	2.03	0.40
1:A:137:TRP:CG	1:A:167:SER:HB2	2.56	0.40

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	82/176 (47%)	79 (96%)	3 (4%)	0	100	100
2	L	215/218 (99%)	208 (97%)	7 (3%)	0	100	100
3	H	208/217 (96%)	200 (96%)	8 (4%)	0	100	100
All	All	505/611 (83%)	487 (96%)	18 (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	76/153 (50%)	74 (97%)	2 (3%)	46	72
2	L	181/182 (100%)	180 (99%)	1 (1%)	86	95
3	H	177/182 (97%)	175 (99%)	2 (1%)	73	89
All	All	434/517 (84%)	429 (99%)	5 (1%)	71	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	SER
1	A	176	MET
2	L	57	SER
3	H	9	ARG
3	H	205	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
3	H	170	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PCA	H	1	3	7,8,9	1.80	1 (14%)	9,10,12	2.11	5 (55%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	H	1	3	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	PCA	CD-N	4.63	1.46	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	PCA	OE-CD-CG	-3.07	121.41	126.76
3	H	1	PCA	CA-N-CD	-2.92	103.60	113.58
3	H	1	PCA	CB-CA-N	2.61	110.80	103.30
3	H	1	PCA	CG-CD-N	2.46	114.75	108.39
3	H	1	PCA	CB-CA-C	-2.23	109.64	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 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, 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	86/176 (48%)	1.65	27 (31%) 0 0	33, 56, 77, 92	0
2	L	217/218 (99%)	0.40	1 (0%) 91 91	18, 32, 51, 82	0
3	H	211/217 (97%)	0.48	8 (3%) 40 43	18, 33, 54, 89	0
All	All	514/611 (84%)	0.64	36 (7%) 16 16	18, 35, 67, 92	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	LYS	5.9
1	A	174	LEU	4.9
1	A	175	ASN	4.9
1	A	178	ALA	4.8
1	A	158	PHE	4.2
3	H	131	SER	4.1
2	L	1	ALA	4.1
1	A	173	ASN	3.7
1	A	184	ARG	3.7
1	A	177	GLU	3.5
1	A	140	TYR	3.4
1	A	142	ILE	3.2
1	A	106	ARG	3.2
1	A	121	THR	3.1
1	A	157	ARG	3.0
1	A	176	MET	2.9
3	H	130	THR	2.9
1	A	201	ARG	2.9
3	H	129	SER	2.8
1	A	179	ASP	2.7
1	A	170	HIS	2.6
1	A	122	ALA	2.6
3	H	62	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	139	TRP	2.5
1	A	191	LYS	2.4
1	A	200	LEU	2.3
1	A	107	VAL	2.3
1	A	130	SER	2.3
3	H	124	ALA	2.3
3	H	214	SER	2.3
3	H	190	THR	2.2
1	A	159	PHE	2.1
1	A	171	ILE	2.1
1	A	185	CYS	2.1
3	H	132	GLY	2.1
1	A	202	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
3	PCA	H	1	8/9	0.95	0.10	36,42,44,54	0

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(Å ²)	Q<0.9
4	CD	L	307	1/1	0.34	0.08	152,152,152,152	0
4	CD	L	305	1/1	0.69	0.12	148,148,148,148	0
4	CD	L	301	1/1	0.73	0.13	139,139,139,139	0
4	CD	L	309	1/1	0.73	0.05	166,166,166,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CD	H	303	1/1	0.75	0.09	190,190,190,190	0
4	CD	A	302	1/1	0.80	0.09	170,170,170,170	0
4	CD	H	301	1/1	0.84	0.08	143,143,143,143	0
4	CD	L	303	1/1	0.85	0.13	98,98,98,98	0
4	CD	L	310	1/1	0.87	0.10	133,133,133,133	0
4	CD	L	308	1/1	0.89	0.18	73,73,73,73	0
4	CD	A	301	1/1	0.95	0.16	72,72,72,72	0
4	CD	L	306	1/1	0.96	0.14	81,81,81,81	0
4	CD	H	302	1/1	0.98	0.10	77,77,77,77	1
4	CD	H	304	1/1	0.98	0.04	141,141,141,141	0
4	CD	L	302	1/1	0.99	0.19	41,41,41,41	0
4	CD	L	304	1/1	0.99	0.15	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.