



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7DAA / pdb_00007daa
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 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
Mogul : 2022.3.0, CSD as543be (2022)
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

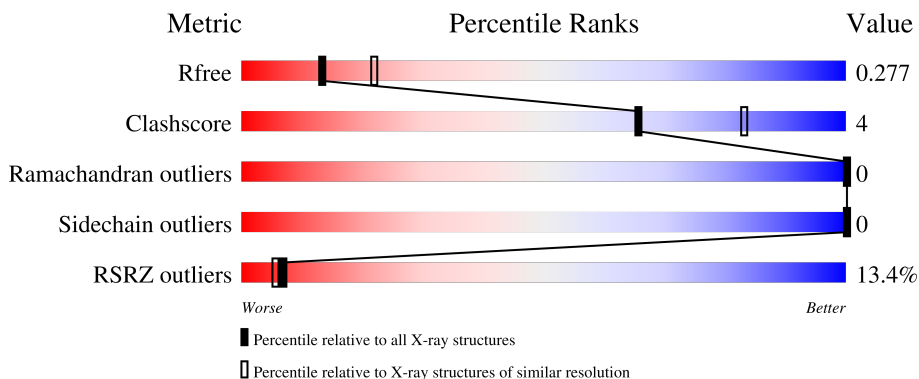
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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	
2	L	218	
3	H	217	

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
			Total	C	N	O	S			
1	A	86	675	419	122	130	4	0	0	0

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
			Total	C	N	O	S			
2	L	217	1630	1022	267	334	7	0	0	0

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

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

- Molecule 4 is CADMIUM ION (CCD ID: 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)	Xtrriage
Refinement program	PHENIX 1.19rc2_4022	Depositor
R, R_{free}	0.228 , 0.283 0.225 , 0.277	Depositor DCC
R_{free} test set	948 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtrriage
Anisotropy	0.087	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.13	0/688	0.30	0/927
2	L	0.13	0/1663	0.30	0/2264
3	H	0.12	0/1597	0.29	0/2187
All	All	0.12	0/3948	0.30	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	11	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	29	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 (29) 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
2:L:193:HIS:C	2:L:194:LYS:HD3	2.44	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 [\(i\)](#)

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	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 [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	76/153 (50%)	76 (100%)	0	100	100
2	L	181/182 (100%)	181 (100%)	0	100	100
3	H	177/182 (97%)	177 (100%)	0	100	100
All	All	434/517 (84%)	434 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	195	GLN
2	L	7	GLN
2	L	23	ASN
2	L	28	GLN
2	L	71	GLN
2	L	141	ASN
3	H	170	GLN
3	H	198	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](#)

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	1.92	1 (14%)	9,10,12	2.14	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	4.95	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	-2.97	121.41	126.72
3	H	1	PCA	CA-N-CD	-2.92	103.60	113.58
3	H	1	PCA	CB-CA-N	2.75	110.80	103.24
3	H	1	PCA	CG-CD-N	2.60	114.75	108.39
3	H	1	PCA	CB-CA-C	-2.20	109.64	112.66

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 oligosaccharides 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%)	2.04	34 (39%) 1 0	33, 56, 77, 92	0
2	L	217/218 (99%)	0.70	19 (8%) 15 14	18, 32, 51, 82	0
3	H	211/217 (97%)	0.72	16 (7%) 20 17	18, 33, 54, 89	0
All	All	514/611 (84%)	0.93	69 (13%) 7 5	18, 35, 67, 92	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	MET	5.0
3	H	132	GLY	5.0
1	A	104	PRO	4.7
1	A	115	HIS	4.7
1	A	191	LYS	4.6
3	H	126	SER	4.6
3	H	214	SER	4.5
1	A	177	GLU	4.3
1	A	106	ARG	4.2
3	H	129	SER	4.1
1	A	203	ARG	3.9
1	A	132	PRO	3.9
2	L	93	TYR	3.8
1	A	141	LYS	3.7
1	A	158	PHE	3.7
3	H	190	THR	3.6
3	H	131	SER	3.6
1	A	171	ILE	3.6
1	A	118	GLU	3.4
3	H	210	VAL	3.3
1	A	189	SER	3.3
1	A	170	HIS	3.3
2	L	1	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
3	H	213	LYS	3.2
2	L	172	SER	3.2
2	L	217	GLU	3.2
2	L	24	CYS	3.2
2	L	132	GLY	3.2
1	A	107	VAL	3.1
1	A	201	ARG	3.1
2	L	58	GLY	3.1
1	A	122	ALA	3.0
1	A	202	VAL	2.9
2	L	33	TYR	2.9
1	A	173	ASN	2.9
1	A	174	LEU	2.9
1	A	183	TYR	2.8
3	H	73	THR	2.8
3	H	130	THR	2.7
1	A	199	THR	2.7
3	H	134	THR	2.6
1	A	124	LEU	2.6
2	L	185	LEU	2.6
1	A	179	ASP	2.6
1	A	185	CYS	2.6
3	H	41	GLY	2.5
1	A	116	ILE	2.5
1	A	190	SER	2.5
2	L	173	LYS	2.5
2	L	149	LYS	2.4
1	A	121	THR	2.4
2	L	133	THR	2.4
1	A	139	TRP	2.4
2	L	57	SER	2.3
2	L	131	SER	2.3
2	L	92	TYR	2.3
1	A	178	ALA	2.2
2	L	130	LYS	2.2
1	A	186	GLN	2.2
3	H	62	ALA	2.1
1	A	109	ALA	2.1
1	A	130	SER	2.1
2	L	175	CYS	2.1
2	L	96	ILE	2.0
2	L	171	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	2.0
3	H	31	TYR	2.0
3	H	97	ALA	2.0
3	H	98	GLY	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	0.91	0.10	36,42,44,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	H	303	1/1	0.73	0.14	190,190,190,190	0
4	CD	L	305	1/1	0.77	0.14	148,148,148,148	0
4	CD	A	302	1/1	0.77	0.18	170,170,170,170	0
4	CD	L	309	1/1	0.78	0.09	166,166,166,166	0
4	CD	L	301	1/1	0.83	0.12	139,139,139,139	0
4	CD	L	310	1/1	0.86	0.15	133,133,133,133	0
4	CD	L	307	1/1	0.86	0.11	152,152,152,152	0
4	CD	L	303	1/1	0.87	0.11	98,98,98,98	0
4	CD	H	301	1/1	0.89	0.09	143,143,143,143	0
4	CD	L	308	1/1	0.94	0.08	73,73,73,73	0
4	CD	H	304	1/1	0.94	0.21	141,141,141,141	0
4	CD	A	301	1/1	0.95	0.06	72,72,72,72	0
4	CD	L	302	1/1	0.96	0.06	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CD	L	306	1/1	0.97	0.09	81,81,81,81	0
4	CD	H	302	1/1	0.97	0.04	77,77,77,77	1
4	CD	L	304	1/1	0.98	0.04	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.