



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3BDY / pdb_00003bdy
Title : Dual specific bH1 Fab in complex with VEGF
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Deposited on : 2007-11-15
Resolution : 2.60 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

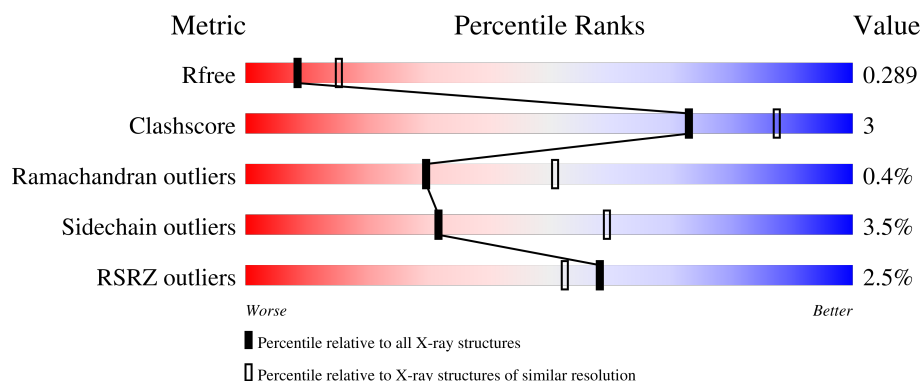
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	H	230	
2	L	218	
3	V	102	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4125 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 Fab Fragment -Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	216	Total	C	N	O	S	0	0	0
			1623	1027	273	317	6			

- Molecule 2 is a protein called Fab Fragment -Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	217	Total	C	N	O	S	0	0	0
			1679	1056	280	338	5			

- Molecule 3 is a protein called Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	95	Total	C	N	O	S	0	0	0
			770	484	130	143	13			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	25	Total	O	0	0
			25	25		
5	L	22	Total	O	0	0
			22	22		

- Molecule 1: Fab Fragment -Heavy Chain



Cluster	Number of Genes
D1	10
D2	10
Q3	10
N4	10
L11	10
T22	10
C23	10
P27C	10
I29	10
Y32	10
W35	10
C68	10
H91	10
Q100	10
E105	10
V110	10
A111	10
P120	10
S121	10
D122	10
V132	10
E143	10
Q147	10
W148	10
L154	10
V163	10
S168	10
S171	10
T172	10
L201	10
V205	10
E213	10
C213	10

GLY	GLN	ASN	HTS	HTS	GLU	V14	D19	Y25	C26	E42	I43	I46	L54	R55	R56	L66	S74	K84	P85	L97	N100	K101	P106	K107	K108	ASP
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	100.60Å 197.98Å 77.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.60) 99.7 (30.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.252 (Not available) , 0.289	Depositor DCC
R_{free} test set	1248 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4125	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: GOL

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	H	0.66	0/1664	0.76	0/2269
2	L	0.64	0/1720	0.76	0/2339
3	V	0.56	0/788	0.70	0/1061
All	All	0.63	0/4172	0.75	0/5669

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	H	1623	0	1577	8	0
2	L	1679	0	1625	11	0
3	V	770	0	741	7	0
4	L	6	0	8	0	0
5	H	25	0	0	0	0
5	L	22	0	0	0	0
All	All	4125	0	3951	26	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 (26) 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:H:20:LEU:HG	1:H:82:MET:HE2	1.78	0.66
2:L:201:LEU:HD13	2:L:205:VAL:HG23	1.84	0.60
1:H:100:PHE:CE2	1:H:101:ALA:HB3	2.40	0.55
2:L:147:GLN:HE21	2:L:154:LEU:HD11	1.73	0.54
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.90	0.53
3:V:74:SER:HB3	3:V:100:ASN:HD21	1.75	0.52
3:V:43:ILE:C	3:V:43:ILE:HD12	2.35	0.52
3:V:56:ARG:NH2	3:V:97:LEU:O	2.43	0.52
1:H:203:LYS:N	1:H:204:PRO:CD	2.73	0.51
2:L:147:GLN:HE22	2:L:154:LEU:HD21	1.74	0.51
1:H:147:TYR:CE1	1:H:152:VAL:HG23	2.46	0.51
3:V:46:ILE:HD12	3:V:85:PRO:HG3	1.92	0.50
2:L:4:MET:HE3	2:L:23:CYS:SG	2.52	0.50
2:L:147:GLN:NE2	2:L:154:LEU:HD11	2.28	0.49
1:H:140:LEU:HD12	1:H:140:LEU:C	2.41	0.46
3:V:25:TYR:O	3:V:26:CYS:C	2.59	0.45
3:V:66:LEU:HD23	3:V:106:PRO:HA	1.99	0.45
2:L:11:LEU:C	2:L:11:LEU:HD12	2.43	0.44
1:H:82:MET:HE1	1:H:111:VAL:HG21	2.00	0.43
1:H:149:PRO:O	1:H:202:HIS:HE1	2.02	0.42
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.53	0.42
1:H:186:VAL:HB	1:H:187:PRO:CD	2.50	0.42
2:L:148:TRP:O	2:L:154:LEU:HD12	2.19	0.41
2:L:32:TYR:HA	2:L:91:HIS:CE1	2.55	0.41
2:L:27(C):PRO:HD2	2:L:29:ILE:HD12	2.01	0.41
3:V:54:LEU:HD13	3:V:56:ARG:NH2	2.36	0.41

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	H	212/230 (92%)	202 (95%)	10 (5%)	0	100	100
2	L	215/218 (99%)	205 (95%)	10 (5%)	0	100	100
3	V	93/102 (91%)	89 (96%)	2 (2%)	2 (2%)	5	10
All	All	520/550 (94%)	496 (95%)	22 (4%)	2 (0%)	30	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	V	26	CYS
3	V	42	GLU

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	H	178/191 (93%)	174 (98%)	4 (2%)	45	72
2	L	191/192 (100%)	183 (96%)	8 (4%)	26	52
3	V	90/96 (94%)	86 (96%)	4 (4%)	25	50
All	All	459/479 (96%)	443 (96%)	16 (4%)	32	59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLU
1	H	129	SER
1	H	153	THR
1	H	163	SER
2	L	2	ILE
2	L	3	GLN
2	L	22	THR
2	L	100	GLN
2	L	105	GLU
2	L	122	ASP
2	L	143	GLU

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Mol	Chain	Res	Type
2	L	163	VAL
3	V	19	ASP
3	V	84	LYS
3	V	101	LYS
3	V	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	39	GLN
1	H	81	GLN
1	H	202	HIS
1	H	206	ASN
2	L	27	GLN
2	L	38	GLN
2	L	124	GLN
2	L	137	ASN
2	L	147	GLN
3	V	87	GLN
3	V	100	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
4	GOL	L	215	-	5,5,5	0.58	0	5,5,5	0.35	0

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
4	GOL	L	215	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	215	GOL	C1-C2-C3-O3
4	L	215	GOL	O2-C2-C3-O3

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	H	216/230 (93%)	0.14	5 (2%) 61 55	36, 46, 57, 72	0
2	L	217/218 (99%)	0.11	7 (3%) 50 44	37, 46, 60, 77	0
3	V	95/102 (93%)	0.12	1 (1%) 78 74	30, 45, 67, 79	0
All	All	528/550 (96%)	0.13	13 (2%) 58 52	30, 46, 60, 79	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	168	SER	3.0
2	L	171	SER	2.8
1	H	215	PRO	2.7
1	H	136	GLY	2.6
1	H	169	PRO	2.6
1	H	0	SER	2.4
2	L	110	VAL	2.4
2	L	100	GLN	2.2
2	L	143	GLU	2.2
3	V	43	ILE	2.2
2	L	172	THR	2.1
2	L	111	ALA	2.0
1	H	175	SER	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](#)

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	GOL	L	215	6/6	0.84	0.20	52,55,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.