



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:25 PM GMT

PDB ID : 1AOX
Title : I DOMAIN FROM INTEGRIN ALPHA2-BETA1
Authors : Emsley, J.; King, S.L.; Bergelson, J.M.; Liddington, R.C.
Deposited on : 1997-07-13
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

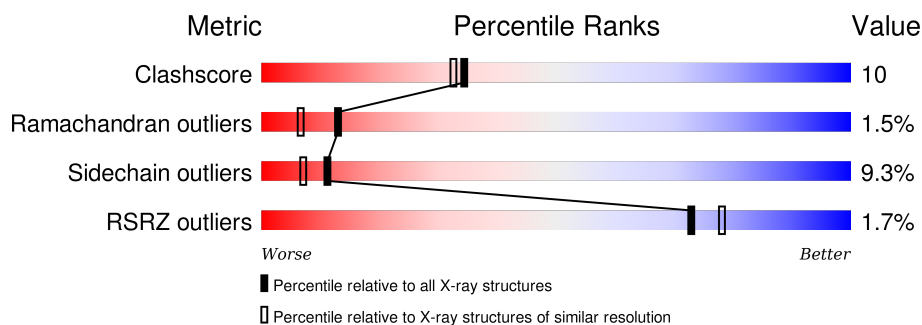
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	203	<div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• • •</div> </div> </div>
1	B	203	<div> <div> <div>2%</div> <div>77%</div> <div>16%</div> <div>5% • •</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3284 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 INTEGRIN ALPHA 2 BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1532	968	256	302	6			
1	B	201	Total	C	N	O	S	0	0	0
			1510	952	256	296	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	DELETION	UNP P17301
A	?	-	PRO	DELETION	UNP P17301
A	?	-	ALA	DELETION	UNP P17301
A	?	-	THR	DELETION	UNP P17301
A	?	-	GLN	DELETION	UNP P17301
A	?	-	PRO	DELETION	UNP P17301
A	337	GLY	-	INSERTION	UNP P17301
B	?	-	PHE	DELETION	UNP P17301
B	?	-	PRO	DELETION	UNP P17301
B	?	-	ALA	DELETION	UNP P17301
B	?	-	THR	DELETION	UNP P17301
B	?	-	GLN	DELETION	UNP P17301
B	?	-	PRO	DELETION	UNP P17301
B	337	GLY	-	INSERTION	UNP P17301

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

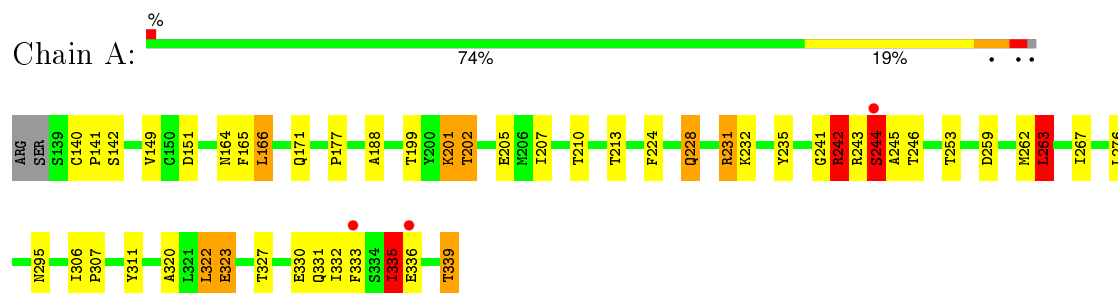
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total 117	O 117	0	0
3	B	123	Total 123	O 123	0	0

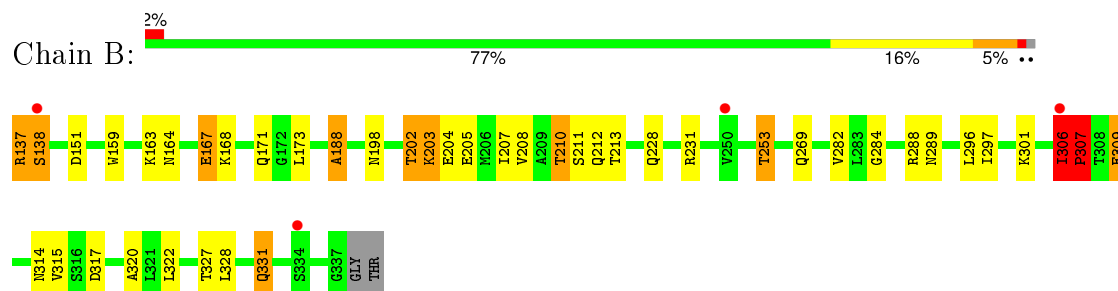
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: INTEGRIN ALPHA 2 BETA



• Molecule 1: INTEGRIN ALPHA 2 BETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.54Å 43.29Å 68.04Å 88.27° 76.59° 66.74°	Depositor
Resolution (Å)	15.00 – 2.10 27.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (15.00-2.10) 94.4 (27.94-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.219 , (Not available) 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 36743 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3284	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.08% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG

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	0.52	1/1557 (0.1%)	0.81	6/2111 (0.3%)
1	B	0.54	0/1534	0.99	4/2086 (0.2%)
All	All	0.53	1/3091 (0.0%)	0.90	10/4197 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	THR	C-OXT	-5.72	1.12	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	ILE	C-N-CD	-20.20	76.17	120.60
1	B	306	ILE	C-N-CA	13.21	177.46	122.00
1	B	307	PRO	CA-N-CD	-6.64	102.20	111.50
1	A	263	LEU	CA-CB-CG	6.18	129.52	115.30
1	A	306	ILE	C-N-CD	-6.17	107.02	120.60
1	B	138	SER	N-CA-C	-5.60	95.88	111.00
1	A	242	ARG	N-CA-C	5.43	125.67	111.00
1	A	244	SER	N-CA-C	-5.39	96.45	111.00
1	A	246	THR	N-CA-C	-5.35	96.55	111.00
1	A	245	ALA	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	306	ILE	Mainchain

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	1532	0	1507	35	0
1	B	1510	0	1464	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	117	0	0	2	0
3	B	123	0	0	2	0
All	All	3284	0	2971	60	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 10.

All (60) 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:B:202:THR:HG22	1:B:205:GLU:H	1.41	0.84
1:A:171:GLN:HB3	1:A:207:ILE:HD11	1.62	0.82
1:A:140:CYS:SG	1:A:244:SER:OG	2.40	0.78
1:A:331:GLN:HA	1:A:331:GLN:NE2	1.99	0.76
1:A:331:GLN:HE21	1:A:331:GLN:HA	1.57	0.69
1:B:315:VAL:HG13	1:B:320:ALA:HB3	1.75	0.68
1:A:202:THR:HB	1:A:205:GLU:HG2	1.74	0.68
1:A:307:PRO:HD2	1:A:311:TYR:HE2	1.58	0.67
1:B:163:LYS:HE2	1:B:211:SER:O	1.95	0.66
1:A:332:ILE:O	1:A:335:ILE:HG22	1.96	0.65
1:A:224:PHE:CZ	1:A:263:LEU:HD23	2.32	0.65
1:A:243:ARG:O	1:A:244:SER:HB3	1.96	0.64
1:B:284:GLY:O	1:B:288:ARG:HG2	1.96	0.64
1:B:171:GLN:HA	1:B:203:LYS:HE3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:PRO:HD2	1:A:311:TYR:CE2	2.34	0.62
1:A:335:ILE:HD12	1:A:336:GLU:N	2.17	0.60
1:A:164:ASN:HB3	1:A:322:LEU:CD1	2.33	0.58
1:B:167:GLU:OE2	1:B:210:THR:HG22	2.04	0.57
1:A:164:ASN:HB3	1:A:322:LEU:HD11	1.87	0.57
1:A:243:ARG:O	1:A:244:SER:CB	2.52	0.57
1:A:339:THR:OXT	1:B:137:ARG:NE	2.38	0.57
1:A:228:GLN:HA	1:A:228:GLN:HE21	1.71	0.55
1:B:297:ILE:CG2	1:B:301:LYS:HE3	2.36	0.55
1:B:163:LYS:O	1:B:167:GLU:HG2	2.08	0.54
1:B:164:ASN:HA	1:B:167:GLU:HG3	1.90	0.53
1:A:231:ARG:NH1	1:A:231:ARG:HG2	2.25	0.52
1:A:141:PRO:O	1:A:142:SER:HB2	2.09	0.52
1:A:333:PHE:HE1	3:A:563:HOH:O	1.93	0.51
1:B:306:ILE:HG22	1:B:307:PRO:HD3	1.93	0.51
1:A:177:PRO:HD3	1:A:201:LYS:HB2	1.93	0.50
1:A:231:ARG:HH11	1:A:231:ARG:CG	2.24	0.50
1:B:208:VAL:O	1:B:212:GLN:HG3	2.12	0.50
1:B:203:LYS:O	1:B:207:ILE:HG12	2.12	0.49
1:A:331:GLN:HE21	1:A:331:GLN:CA	2.20	0.48
1:A:259:ASP:O	1:A:262:MET:HG2	2.13	0.48
1:A:235:TYR:O	1:A:241:GLY:HA3	2.14	0.48
1:A:320:ALA:O	1:A:323:GLU:HG3	2.14	0.48
1:A:231:ARG:NH1	1:A:231:ARG:CG	2.76	0.47
1:B:297:ILE:HG22	1:B:301:LYS:HE3	1.96	0.47
1:A:332:ILE:O	1:A:335:ILE:CG2	2.63	0.47
1:A:141:PRO:HD3	1:B:137:ARG:NH1	2.30	0.47
1:A:262:MET:HB3	3:A:626:HOH:O	2.14	0.46
1:B:188:ALA:HB3	3:B:736:HOH:O	2.16	0.46
1:B:228:GLN:HA	1:B:231:ARG:HG2	1.96	0.46
1:A:210:THR:O	1:A:213:THR:HG22	2.16	0.46
1:B:159:TRP:HE1	1:B:213:THR:HG23	1.80	0.45
1:B:309:GLU:CD	1:B:309:GLU:H	2.20	0.45
1:B:228:GLN:NE2	1:B:269:GLN:OE1	2.51	0.44
1:B:151:ASP:HB2	1:B:253:THR:HA	1.99	0.44
1:B:327:THR:O	1:B:331:GLN:HB2	2.18	0.43
1:B:202:THR:HG23	1:B:204:GLU:H	1.82	0.43
1:A:327:THR:HA	1:A:330:GLU:HG2	2.01	0.43
1:B:168:LYS:NZ	3:B:621:HOH:O	2.51	0.43
1:B:289:ASN:HD22	1:B:289:ASN:HA	1.61	0.42
1:B:137:ARG:C	1:B:138:SER:O	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASP:HB2	1:A:253:THR:HA	2.02	0.42
1:B:173:LEU:O	1:B:203:LYS:NZ	2.54	0.41
1:A:224:PHE:HZ	1:A:263:LEU:HD23	1.84	0.41
1:A:242:ARG:O	1:A:243:ARG:CB	2.69	0.41
1:A:165:PHE:CD2	1:A:166:LEU:HD13	2.57	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	A	199/203 (98%)	187 (94%)	8 (4%)	4 (2%)	9	4
1	B	199/203 (98%)	192 (96%)	5 (2%)	2 (1%)	19	13
All	All	398/406 (98%)	379 (95%)	13 (3%)	6 (2%)	13	7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	307	PRO
1	A	244	SER
1	A	188	ALA
1	B	188	ALA
1	A	199	THR
1	A	335	ILE

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	165/170 (97%)	150 (91%)	15 (9%)	12	7
1	B	159/170 (94%)	144 (91%)	15 (9%)	11	7
All	All	324/340 (95%)	294 (91%)	30 (9%)	11	7

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	VAL
1	A	166	LEU
1	A	201	LYS
1	A	202	THR
1	A	228	GLN
1	A	231	ARG
1	A	232	LYS
1	A	242	ARG
1	A	263	LEU
1	A	267	ILE
1	A	276	LEU
1	A	295	ASN
1	A	322	LEU
1	A	323	GLU
1	A	335	ILE
1	B	137	ARG
1	B	167	GLU
1	B	198	ASN
1	B	202	THR
1	B	203	LYS
1	B	210	THR
1	B	253	THR
1	B	282	VAL
1	B	296	LEU
1	B	309	GLU
1	B	314	ASN
1	B	317	ASP
1	B	322	LEU
1	B	328	LEU
1	B	331	GLN

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

Mol	Chain	Res	Type
1	A	228	GLN
1	A	287	ASN
1	A	295	ASN
1	A	314	ASN
1	A	331	GLN
1	B	198	ASN
1	B	228	GLN
1	B	287	ASN
1	B	289	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 ⓘ

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	A	201/203 (99%)	-0.18	3 (1%) 76 81	12, 30, 59, 80	0
1	B	201/203 (99%)	-0.31	4 (1%) 68 73	11, 26, 45, 60	0
All	All	402/406 (99%)	-0.25	7 (1%) 73 78	11, 28, 52, 80	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	SER	5.7
1	A	333	PHE	3.7
1	B	334	SER	3.4
1	B	306	ILE	2.5
1	A	336	GLU	2.1
1	B	138	SER	2.1
1	B	250	VAL	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	A	400	1/1	0.99	0.06	-2.38	19,19,19,19	0
2	MG	B	401	1/1	0.99	0.06	-2.90	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.