



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 26, 2018 – 07:13 AM EDT

PDB ID : 1RD4
Title : An allosteric inhibitor of LFA-1 bound to its I-domain
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Deposited on : 2003-11-05
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031021

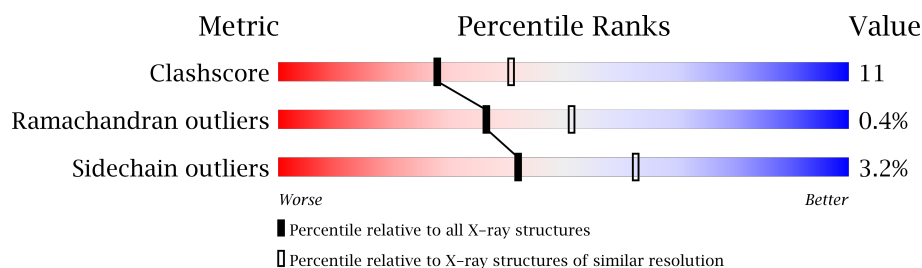
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	191	
1	B	191	
1	C	191	
1	D	191	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6052 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.

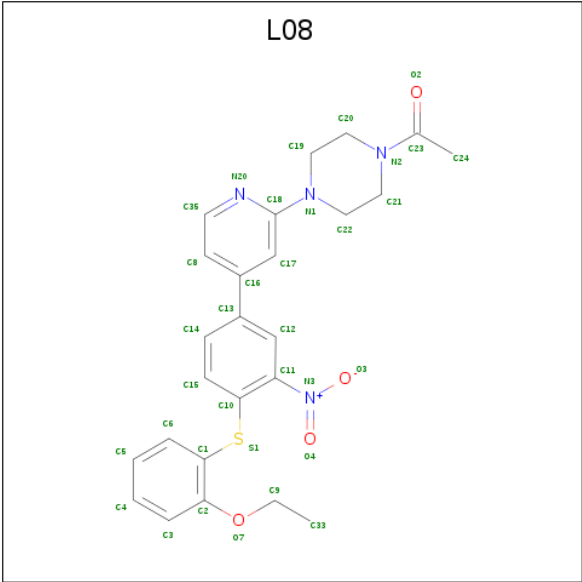
- Molecule 1 is a protein called Integrin alpha-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1479	956	236	283	4			
1	B	184	Total	C	N	O	S	0	0	0
			1479	956	236	283	4			
1	C	184	Total	C	N	O	S	0	0	0
			1479	956	236	283	4			
1	D	184	Total	C	N	O	S	0	0	0
			1479	956	236	283	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	GLY	-	CLONING ARTIFACT	UNP P20701
A	122	ALA	-	CLONING ARTIFACT	UNP P20701
A	123	MET	-	CLONING ARTIFACT	UNP P20701
A	124	SER	-	CLONING ARTIFACT	UNP P20701
B	121	GLY	-	CLONING ARTIFACT	UNP P20701
B	122	ALA	-	CLONING ARTIFACT	UNP P20701
B	123	MET	-	CLONING ARTIFACT	UNP P20701
B	124	SER	-	CLONING ARTIFACT	UNP P20701
C	121	GLY	-	CLONING ARTIFACT	UNP P20701
C	122	ALA	-	CLONING ARTIFACT	UNP P20701
C	123	MET	-	CLONING ARTIFACT	UNP P20701
C	124	SER	-	CLONING ARTIFACT	UNP P20701
D	121	GLY	-	CLONING ARTIFACT	UNP P20701
D	122	ALA	-	CLONING ARTIFACT	UNP P20701
D	123	MET	-	CLONING ARTIFACT	UNP P20701
D	124	SER	-	CLONING ARTIFACT	UNP P20701

- Molecule 2 is 1-ACETYL-4-(4-{4-[(2-ETHOXYPHENYL)THIO]-3-NITROPHENYL}PYRIDIN-2-YL)PIPERAZINE (three-letter code: L08) (formula: C₂₅H₂₆N₄O₄S).



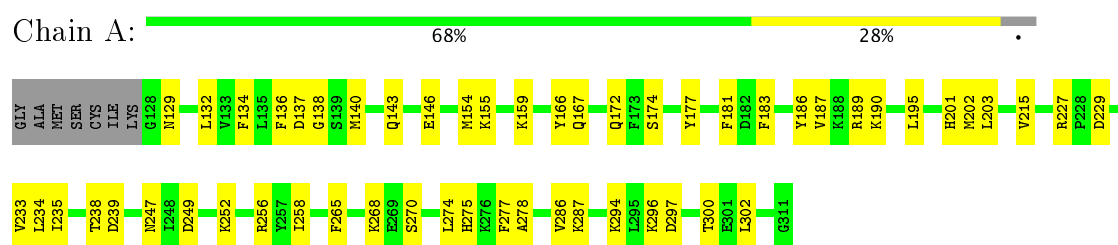
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	25	4	4	1		
2	B	1	Total	C	N	O	S	0	0
			34	25	4	4	1		
2	C	1	Total	C	N	O	S	0	0
			34	25	4	4	1		
2	D	1	Total	C	N	O	S	0	0
			34	25	4	4	1		

3 Residue-property plots [i](#)

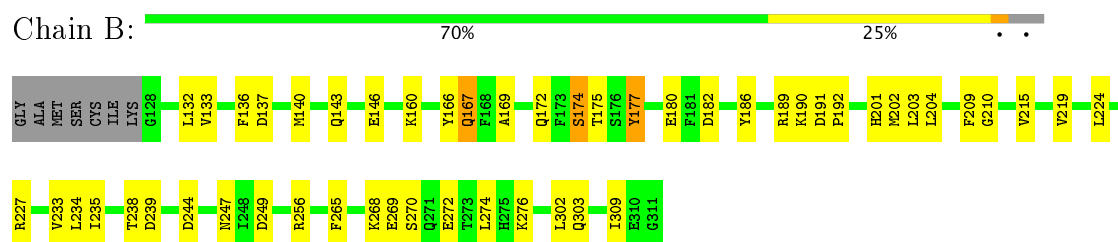
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

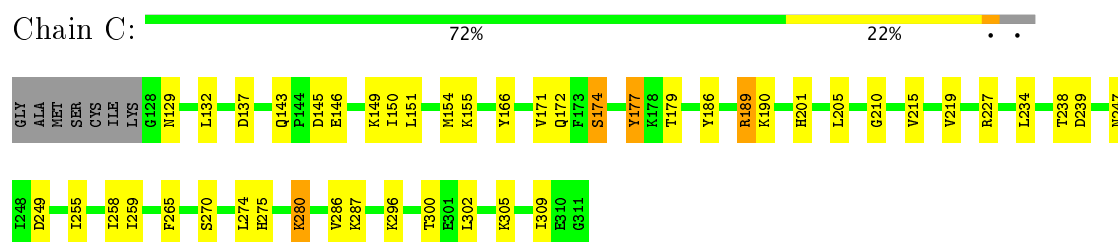
- Molecule 1: Integrin alpha-L



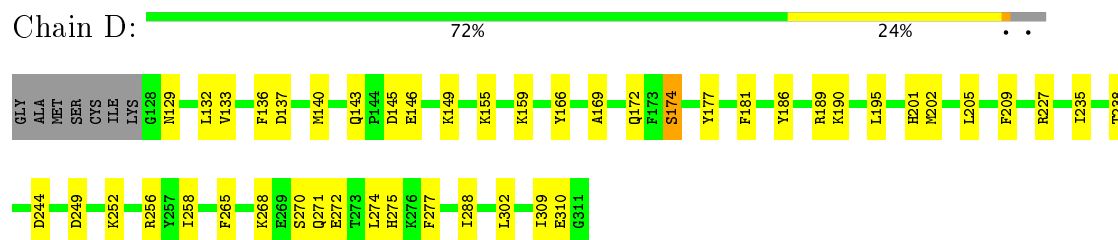
- Molecule 1: Integrin alpha-L



- Molecule 1: Integrin alpha-L



- Molecule 1: Integrin alpha-L



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.96 Å 64.41 Å 66.21 Å 74.21° 90.00° 87.26°	Depositor
Resolution (Å)	40.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6052	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: L08

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	0.45	0/1507	0.60	0/2026
1	B	0.45	0/1507	0.58	0/2026
1	C	0.45	0/1507	0.60	0/2026
1	D	0.45	0/1507	0.59	0/2026
All	All	0.45	0/6028	0.59	0/8104

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 [i](#)

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	1479	0	1487	35	0
1	B	1479	0	1487	34	0
1	C	1479	0	1487	35	0
1	D	1479	0	1487	26	0
2	A	34	0	26	2	0
2	B	34	0	26	3	0
2	C	34	0	26	5	0
2	D	34	0	26	2	0
All	All	6052	0	6052	130	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 11.

The worst 5 of 130 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:132:LEU:HD11	1:A:235:ILE:HD11	1.46	0.96
1:C:309:ILE:HD13	1:D:309:ILE:HD13	1.48	0.95
1:B:132:LEU:HD21	1:B:235:ILE:HD12	1.64	0.78
1:D:268:LYS:O	1:D:272:GLU:HG2	1.83	0.78
1:B:132:LEU:HD11	1:B:235:ILE:HD11	1.64	0.77

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	182/191 (95%)	171 (94%)	11 (6%)	0	100	100
1	B	182/191 (95%)	170 (93%)	11 (6%)	1 (0%)	31	44
1	C	182/191 (95%)	171 (94%)	10 (6%)	1 (0%)	31	44
1	D	182/191 (95%)	171 (94%)	10 (6%)	1 (0%)	31	44
All	All	728/764 (95%)	683 (94%)	42 (6%)	3 (0%)	36	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	174	SER
1	B	174	SER
1	C	174	SER

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	163/168 (97%)	158 (97%)	5 (3%)	43	64
1	B	163/168 (97%)	157 (96%)	6 (4%)	37	56
1	C	163/168 (97%)	157 (96%)	6 (4%)	37	56
1	D	163/168 (97%)	159 (98%)	4 (2%)	50	71
All	All	652/672 (97%)	631 (97%)	21 (3%)	42	62

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	276	LYS
1	C	177	TYR
1	D	140	MET
1	B	269	GLU
1	D	177	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	163	ASN
1	C	172	GLN
1	D	163	ASN
1	B	303	GLN
1	D	172	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are 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$
2	L08	A	328	-	36,37,37	3.75	25 (69%)	45,51,51	2.47	14 (31%)
2	L08	B	1328	-	36,37,37	3.50	23 (63%)	45,51,51	2.57	17 (37%)
2	L08	C	2328	-	36,37,37	3.70	24 (66%)	45,51,51	2.44	15 (33%)
2	L08	D	3328	-	36,37,37	3.58	24 (66%)	45,51,51	2.57	16 (35%)

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
2	L08	A	328	-	-	0/21/33/33	0/4/4/4
2	L08	B	1328	-	-	0/21/33/33	0/4/4/4
2	L08	C	2328	-	-	0/21/33/33	0/4/4/4
2	L08	D	3328	-	-	2/21/33/33	0/4/4/4

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	328	L08	C1-S1	-2.13	1.75	1.78
2	D	3328	L08	C18-N20	-2.02	1.29	1.34
2	B	1328	L08	C10-S1	2.07	1.81	1.78
2	B	1328	L08	C22-C21	2.08	1.59	1.51
2	D	3328	L08	C23-N2	2.08	1.41	1.35

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3328	L08	C21-N2-C23	-5.89	107.34	122.93
2	C	2328	L08	C21-N2-C23	-5.59	108.13	122.93
2	A	328	L08	C21-N2-C23	-5.57	108.18	122.93
2	D	3328	L08	C12-C11-C10	-5.48	117.28	122.96
2	B	1328	L08	C21-N2-C23	-5.42	108.58	122.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3328	L08	C24-C23-N2-C21
2	D	3328	L08	O2-C23-N2-C21

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	328	L08	2	0
2	B	1328	L08	3	0
2	C	2328	L08	5	0
2	D	3328	L08	2	0

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.