



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:34 AM GMT

PDB ID : 1EZU
Title : ECOTIN Y69F, D70P BOUND TO D102N TRYPSIN
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Deposited on : 2000-05-11
Resolution : 2.40 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

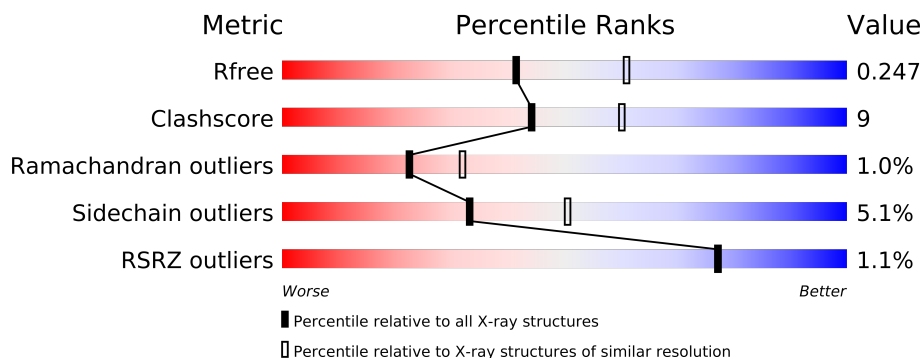
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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))
R_{free}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	142	
1	B	142	
2	C	223	
2	D	223	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5554 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ECOTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1099	704	182	207	6			
1	B	140	Total	C	N	O	S	0	0	0
			1099	704	182	207	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	PHE	TYR	ENGINEERED	UNP P23827
A	70	PRO	ASP	ENGINEERED	UNP P23827
B	269	PHE	TYR	ENGINEERED	UNP P23827
B	270	PRO	ASP	ENGINEERED	UNP P23827

- Molecule 2 is a protein called TRYPSIN II, ANIONIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	223	Total	C	N	O	S	0	0	0
			1656	1036	281	325	14			
2	D	223	Total	C	N	O	S	0	0	0
			1656	1036	281	325	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	479	ASP	ASN	SEE REMARK 999	UNP P00763
C	502	ASN	ASP	ENGINEERED	UNP P00763
D	779	ASP	ASN	SEE REMARK 999	UNP P00763
D	802	ASN	ASP	ENGINEERED	UNP P00763

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	9	Total	O	0	0
			9	9		
4	C	12	Total	O	0	0
			12	12		
4	D	12	Total	O	0	0
			12	12		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.92Å 82.75Å 81.75Å 90.00° 97.24° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 26.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.5 (25.00-2.40) 92.6 (26.50-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , 0.265 0.213 , 0.247	Depositor DCC
R_{free} test set	1508 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 24.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30238 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5554	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.56	0/1122	0.78	1/1521 (0.1%)
1	B	0.55	0/1122	0.78	0/1521
2	C	0.54	0/1691	0.73	1/2306 (0.0%)
2	D	0.53	0/1691	0.74	2/2306 (0.1%)
All	All	0.54	0/5626	0.75	4/7654 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	899	VAL	N-CA-C	-5.50	96.14	111.00
1	A	81	VAL	N-CA-C	-5.45	96.27	111.00
2	C	437	SER	N-CA-C	-5.20	96.95	111.00
2	D	837	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1099	0	1095	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1099	0	1095	13	0
2	C	1656	0	1586	28	0
2	D	1656	0	1586	41	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	9	0	0	1	0
4	B	9	0	0	0	0
4	C	12	0	0	1	0
4	D	12	0	0	1	0
All	All	5554	0	5362	94	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 94 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:86:ALA:HB3	2:D:741:PHE:HA	1.73	0.70
1:A:53:HIS:CD2	1:A:82:SER:HB3	2.27	0.70
2:D:824:PRO:HG3	2:D:909:LEU:O	1.93	0.68
1:A:133:GLU:HG2	1:B:329:VAL:O	1.97	0.64
2:D:772:ASN:HD22	2:D:774:ASN:H	1.44	0.63

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	138/142 (97%)	131 (95%)	5 (4%)	2 (1%)	16	22
1	B	138/142 (97%)	135 (98%)	2 (1%)	1 (1%)	30	43
2	C	221/223 (99%)	204 (92%)	14 (6%)	3 (1%)	16	22
2	D	221/223 (99%)	207 (94%)	13 (6%)	1 (0%)	38	53
All	All	718/730 (98%)	677 (94%)	34 (5%)	7 (1%)	22	32

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	PRO
1	B	288	PRO
2	C	449	ASP
2	D	749	ASP
1	A	49	ASP

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	119/125 (95%)	113 (95%)	6 (5%)	34	51
1	B	119/125 (95%)	113 (95%)	6 (5%)	34	51
2	C	183/185 (99%)	175 (96%)	8 (4%)	39	58
2	D	183/185 (99%)	172 (94%)	11 (6%)	27	41
All	All	604/620 (97%)	573 (95%)	31 (5%)	33	50

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	475	VAL
2	C	490	LYS
2	D	837	LEU
2	C	476	LEU
2	C	518	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	481	GLN
2	C	550	ASN
2	D	781	GLN
2	C	472	ASN
2	D	772	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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.

5.7 Other polymers ⓘ

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

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	140/142 (98%)	-0.31	4 (2%) 49 47	20, 44, 73, 100	0
1	B	140/142 (98%)	-0.40	0 100 100	24, 44, 74, 99	0
2	C	223/223 (100%)	-0.39	0 100 100	16, 38, 61, 85	0
2	D	223/223 (100%)	-0.24	4 (1%) 65 63	20, 40, 69, 96	0
All	All	726/730 (99%)	-0.33	8 (1%) 77 77	16, 42, 71, 100	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	SER	5.4
2	D	777	GLU	4.8
1	A	4	VAL	4.8
2	D	778	GLY	3.4
2	D	847	SER	2.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	C	650	1/1	0.06	-	47,47,47,47	0
3	CA	D	950	1/1	0.10	-	80,80,80,80	0

6.5 Other polymers ⓘ

There are no such residues in this entry.