wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:04 PM GMT

PDB ID	:	1DT5
Title	:	THE STRUCTURAL ORIGINS OF INTERFACIAL ACTIVATION IN THERMOMYCES (HUMICOLA) LANUGINOSA LIPASE
Authors	:	Brozozowski, A.M.; Savage, H.
Deposited on	:	2000-01-11
Resolution	:	2.40 Å(reported)

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

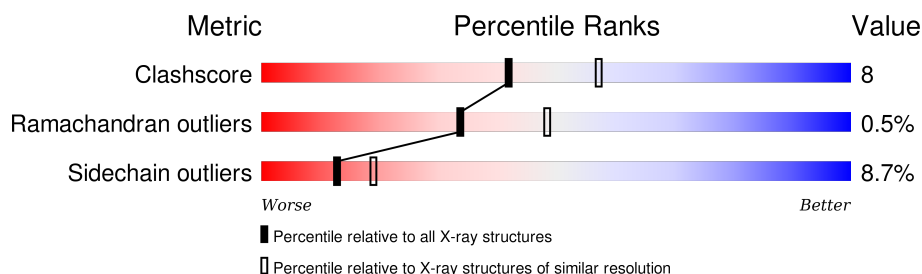|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		0.5%
Sidechain outliers		8.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	269	77% 17% 5% •
1	B	269	76% 17% 6% •
1	C	269	76% 20% • •
1	D	269	77% 17% 5% •
1	E	269	76% 19% • •
1	F	269	75% 20% • •
1	G	269	71% 22% 6% •

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Mol	Chain	Length	Quality of chain
1	H	269	

76%　　　19%　　　5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17081 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 LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	B	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	C	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	D	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	E	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	F	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	G	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	H	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total	O	0	0
			90	90		
2	B	102	Total	O	0	0
			102	102		
2	C	64	Total	O	0	0
			64	64		
2	D	68	Total	O	0	0
			68	68		
2	E	57	Total	O	0	0
			57	57		
2	F	51	Total	O	0	0
			51	51		

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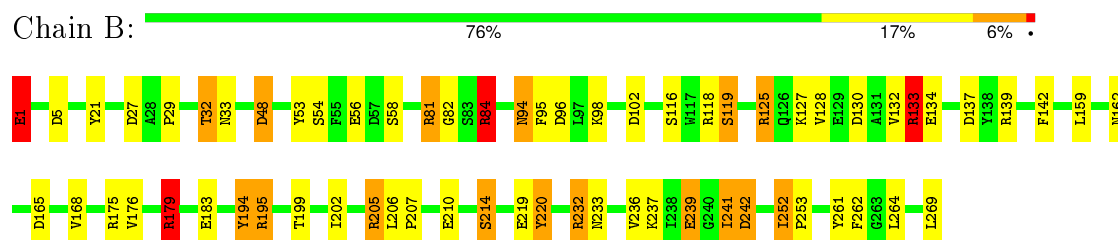| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	30	Total 30	O 30	0	0
2	H	51	Total 51	O 51	0	0

3 Residue-property plots ⓘ

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 (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.
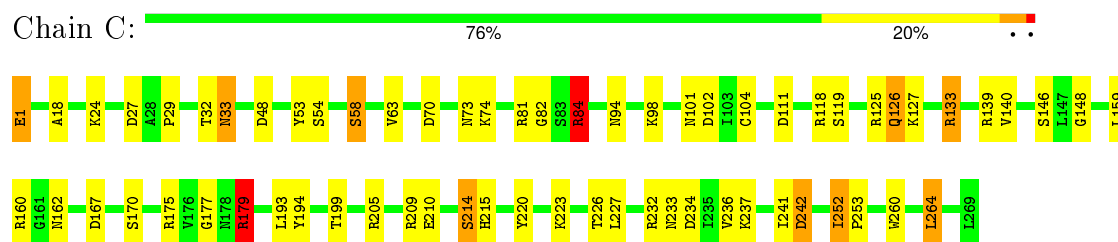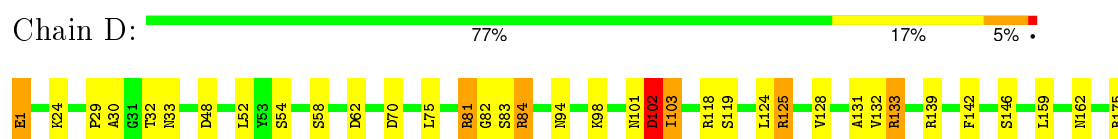
Note EDS was not executed.
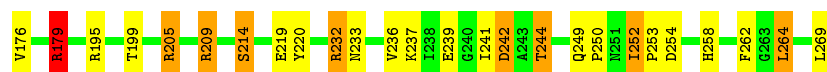
- Molecule 1: LIPASE

Chain A:

- Molecule 1: LIPASE

Chain B:

- Molecule 1: LIPASE

Chain C:

- Molecule 1: LIPASE

Chain D:

V176 R179 R195 T199 R205 R209 S214 E219 Y220 R232 N233 V236 K237 I238 E239 G240 I241 D242 A243 T244 Q249 P250 N251 I252 P253 D254 H258 F262 G263 L264 L269

• Molecule 1: LIPASE

Chain E:

76% 19% • •

E1 D5 Q15 A20 Y21 K24 P29 N33 C36 T37 A40 E43 D48 Y53 S54 S58 R81 G82 S83 R84 W89 N94 F95 D102 R118 S119 R125 Q126 K127 R133 R139 F142 S146 L147 L159

N162 V168 V176 R179 V187 Y194 R195 T199 N200 V203 P204 R205 L206 P207 P208 R209 E210 F211 S214 R232 N233 V236 E239 G240 I241 D242 Q249 I252 P253 D254 F262 G263 L264 L269

• Molecule 1: LIPASE

Chain F:

75% 20% • •

E1 Q15 A20 N26 P29 T32 N33 I34 T37 C41 Y53 S54 F55 E56 D57 S58 G59 V60 V63 D70 N73 K74 R81 G82 S83 R84 N94 F95 D102 S116 W117 R118 S119 L124 R125 Q126 K127 V128 V132 R133 R139

S146 L159 R160 G161 N162 F169 S170 Y171 R175 V176 R179 R195 T199 N200 D201 P204 R205 L206 P207 P208 R209 E210 Y213 S214 S224 R232 I241 D242 G245 I252 P253 D254 Y261 F262 G263 L264 L269

• Molecule 1: LIPASE

Chain G:

71% 22% 6% •

E1 A20 N25 A28 P29 T32 N33 I34 D48 F51 L52 Y53 S54 S58 V63 L67 N73 K74 R81 R84 N94 F95 D96 D102 R118 S119 V120 A121 L124 R125 Q126 K127 V128 R133 R139 V140 V141 S146 L147 V154

L159 R160 G161 N162 G163 Y164 V168 Y171 V176 R179 E183 T186 R195 H198 T199 N200 D201 I202 R205 L206 P207 P208 R209 S214 S217 P218 E219 Y220 W221 I222 K223 S224 L227 R232 K237 G240 I241 D242 A243 T252 P253 D254 I255

P256 W260 Y261 F262 G263 L264 L269

• Molecule 1: LIPASE

Chain H:

76% 19% 5% •

E1 A20 P29 T32 N33 N39 D48 A49 S58 V63 T64 L69 N73 K74 L78 R81 G82 S83 R84 N94 E99 D102 R108 D111 S116 W117 R118 S119 R125 Q126 K127 R133 F142 S146 L159 R160 G161 N162

I166 R175 V176 R179 E183 G191 R195 T199 P204 R205 L206 P207 P208 R209 E210 S214 E219 K223 T226 L227 R232 I235 V236 I241 D242 N247 I252 P253 Y261 F262 G263 L264 L269

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.44Å 162.88Å 86.72Å 90.00° 98.45° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	98.4 (20.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.244 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17081	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.67	0/2121	1.67	38/2887 (1.3%)
1	B	0.69	1/2121 (0.0%)	1.74	39/2887 (1.4%)
1	C	0.57	0/2121	1.54	27/2887 (0.9%)
1	D	0.60	0/2121	1.59	30/2887 (1.0%)
1	E	0.54	0/2121	1.55	32/2887 (1.1%)
1	F	0.56	0/2121	1.55	29/2887 (1.0%)
1	G	0.52	0/2121	1.42	20/2887 (0.7%)
1	H	0.55	0/2121	1.52	21/2887 (0.7%)
All	All	0.59	1/16968 (0.0%)	1.58	236/23096 (1.0%)

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	A	0	8
1	B	0	3
1	C	0	6
1	D	0	5
1	E	0	4
1	F	0	4
1	G	0	7
1	H	0	2
All	All	0	39

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	ARG	CD-NE	-5.61	1.36	1.46

The worst 5 of 236 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	205	ARG	CD-NE-CZ	25.18	158.84	123.60
1	H	205	ARG	CD-NE-CZ	24.04	157.25	123.60
1	F	205	ARG	NE-CZ-NH1	21.41	131.00	120.30
1	D	205	ARG	CD-NE-CZ	21.20	153.28	123.60
1	E	205	ARG	NE-CZ-NH2	-20.43	110.08	120.30

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	LEU	Mainchain
1	A	15	GLN	Mainchain
1	A	151	LEU	Mainchain
1	A	168	VAL	Mainchain
1	A	45	GLU	Mainchain

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	2071	0	1965	30	0
1	B	2071	0	1965	31	0
1	C	2071	0	1965	26	0
1	D	2071	0	1965	41	1
1	E	2071	0	1965	33	1
1	F	2071	0	1965	32	0
1	G	2071	0	1965	50	0
1	H	2071	0	1965	37	0
2	A	90	0	0	5	1
2	B	102	0	0	6	1
2	C	64	0	0	4	0
2	D	68	0	0	10	0
2	E	57	0	0	5	0
2	F	51	0	0	5	0
2	G	30	0	0	9	0
2	H	51	0	0	6	0
All	All	17081	0	15720	271	2

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 8.

The worst 5 of 271 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:231:THR:HG21	1:G:125:ARG:HH12	1.21	1.02
1:F:252:ILE:HD12	1:F:253:PRO:HD2	1.50	0.94
1:D:252:ILE:HD12	1:D:253:PRO:HD2	1.52	0.92
1:H:252:ILE:HD12	1:H:253:PRO:HD2	1.51	0.92
1:H:179:ARG:NH2	2:H:270:HOH:O	2.03	0.91

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:311:HOH:O	2:B:361:HOH:O[2_546]	1.97	0.23
1:D:102:ASP:O	1:E:232:ARG:NH2[2_657]	2.13	0.07

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	267/269 (99%)	256 (96%)	10 (4%)	1 (0%)	39	56
1	B	267/269 (99%)	257 (96%)	9 (3%)	1 (0%)	39	56
1	C	267/269 (99%)	255 (96%)	11 (4%)	1 (0%)	39	56
1	D	267/269 (99%)	256 (96%)	8 (3%)	3 (1%)	17	25
1	E	267/269 (99%)	254 (95%)	12 (4%)	1 (0%)	39	56
1	F	267/269 (99%)	256 (96%)	10 (4%)	1 (0%)	39	56
1	G	267/269 (99%)	256 (96%)	10 (4%)	1 (0%)	39	56
1	H	267/269 (99%)	257 (96%)	9 (3%)	1 (0%)	39	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2136/2152 (99%)	2047 (96%)	79 (4%)	10 (0%)	34 48

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	102	ASP
1	A	199	THR
1	E	199	THR
1	H	199	THR
1	C	199	THR

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	220/220 (100%)	202 (92%)	18 (8%)	14	21
1	B	220/220 (100%)	199 (90%)	21 (10%)	11	15
1	C	220/220 (100%)	202 (92%)	18 (8%)	14	21
1	D	220/220 (100%)	199 (90%)	21 (10%)	11	15
1	E	220/220 (100%)	201 (91%)	19 (9%)	13	19
1	F	220/220 (100%)	201 (91%)	19 (9%)	13	19
1	G	220/220 (100%)	203 (92%)	17 (8%)	16	24
1	H	220/220 (100%)	200 (91%)	20 (9%)	12	17
All	All	1760/1760 (100%)	1607 (91%)	153 (9%)	13	19

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	162	ASN
1	E	118	ARG
1	H	119	SER
1	D	179	ARG
1	D	269	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	33	ASN
1	E	26	ASN
1	F	33	ASN
1	C	33	ASN
1	E	33	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)

There are no ligands in this entry.

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)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.