

SUPPLEMENTARY MATERIALS:

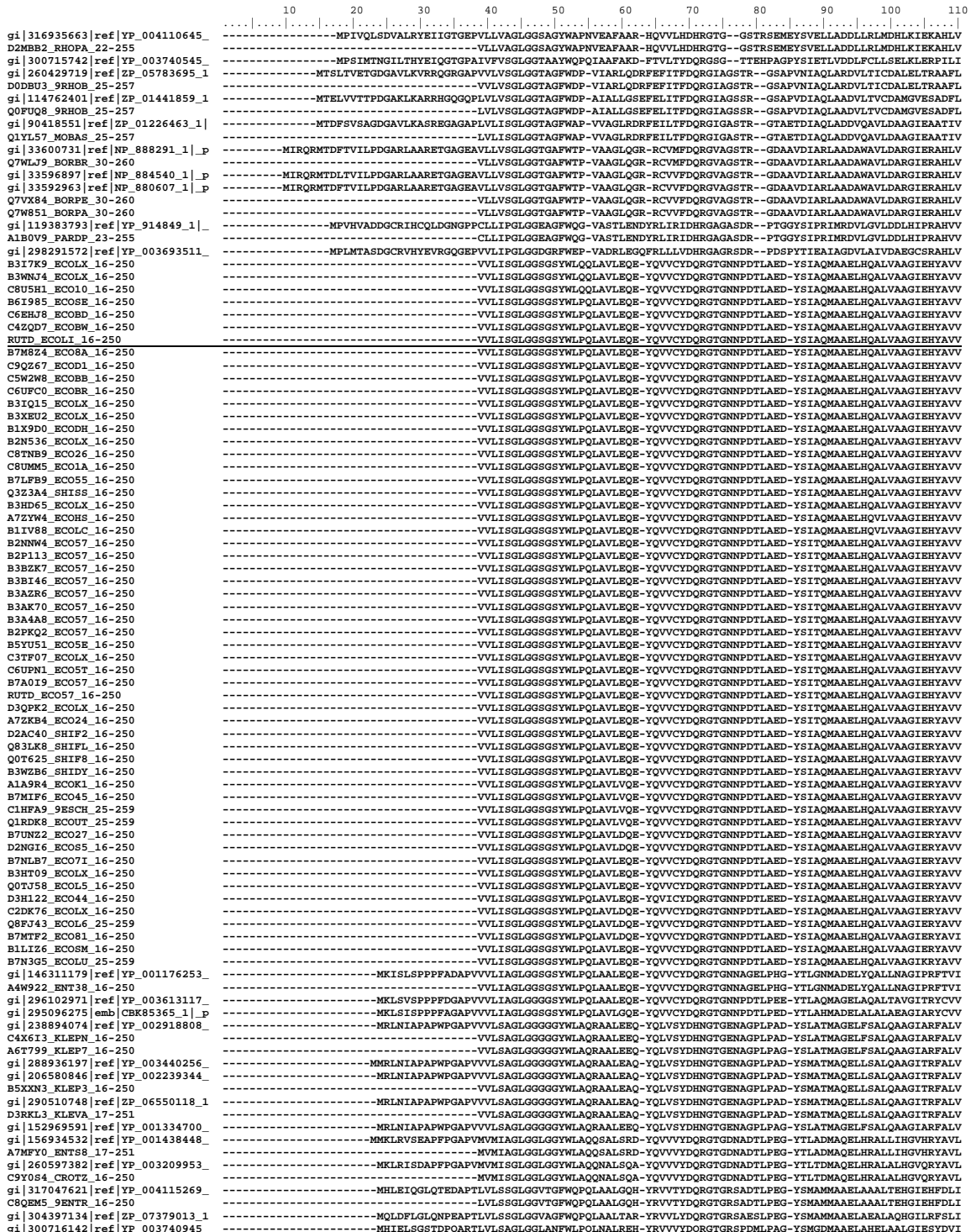
Table S1.

Summary of X-ray data and model parameters of RutD protein

Summary of Crystallographic Information	
A. Data Collection and Phasing	
Beamline	21 ID-F ANL
Wavelength (Å)	0.9787
Space group	P4 ₁ 2 ₁ 2
Resolution range (Å)	50.00-2.10 (2.10-2.14)
Unit cell parameters	
Length (Å)	a = 79.6 b = 79.6 c = 161.8
Angles (°)	$\alpha = \beta = \gamma = 90$
Wilson plot B (Å²)	25.1
R_{merge}	0.357*
I/σ(I)	11.6 (2.9)
Completeness (%)	98.0 (95.0)
Redundancy	10.2 (8.4)
No. of observations	315760
No of unique reflections	19039 (898)
Figure of merit for SAD phasing (after DM)	0.808
B. Refinement	
R_{work}/R_{free} (%)	16.9/22.6
No. of protein atoms	4060 (37.6)
(B-factor, Å²)	
No. of solvent atoms	313 (41.7)
(B-factor, Å²)	
No. of ligand atoms	33 (42.3)
(B-factor, Å²)	
R.m.s. deviations	
Bond lengths (Å)	0.013
Bond angles (°)	1.5
Ramachandran plot	
Most favored (%)	98.86
Allowed (%)	1.14
Disallowed (%)	0

* High value of R_{merge} is caused by multiple crystal lattices (Supplementary figure S3). When corrections for radiation decay and anisotropic diffraction are applied^{40,41} the traditional crystallographic parameters are not the best to describe the quality of the diffraction data. Despite the very high R_{merge} the R, R_{free}, and geometrical parameters obtained after structure refinement are significantly better than for other structures deposited to PDB during the last two years.

Fig.S1. Multiple sequence alignment of protein sequences belonging to the RutD family, obtained by CLANS clustering. 100% conserved putative active site residues are highlighted: H87 and H237 in magenta, R128 in blue, and D209 in red (following the RutD sequence numbering). The residue C-terminal to H87 is also highlighted: A in teal, and S in grey. The RutD sequence is underscored.



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A8IAD8_AZOC5_22-255 -----VLSAGMGGGAPFWPQTEALAAH-HQVILYDHAGTGRSAGVTPSG-YTLADMADELADLALASQHTIERHYFV

120 130 140 150 160 170 180 190 200 210 220
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GHS TGGAMGIVLGAQAP-----ERIASLVLYATWAEIDQMBESCSILRRLLRGMGEAEYHRAATPLFLYPPYMRDHKADLEREVAALIAATPSSRIMDARAAGIMAFDGLR
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gi|260429719|ref|ZP_05783695_1|... GHS TGGCIVQTLAATAP-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
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GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
gi|B3XRU2_ECOLX_16-250... GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
gi|B1X9D0_ECOHD_16-250... GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
gi|B2N536_ECOLX_16-250... GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
gi|C8TNB9_ECO26_16-250... GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
gi|C8UMM5_ECO1A_16-250... GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
gi|B7LFB9_ECO55_16-250... GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
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gi|B4ZYW4_ECOHS_16-250... GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
gi|B1V988_ECOLC_16-250... GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
gi|B2N1M4_ECO57_16-250... GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
gi|B3BZK7_ECO57_16-250... GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
gi|B3B146_ECO57_16-250... GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
gi|B3AZR6_ECO57_16-250... GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
gi|B3AK70_ECO57_16-250... GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG
GHS TGGCIVQTLAATA-----SERVERLALSAAWIKPGNYLITALFELRGLLHRD-PRAYAESALLSYAPGWLSEHWKCYERATANPADPQKVAIVRILVLDGFSG

gi | 289626193 | ref | ZP_06459147_1 | SLARIQT--PTLLIANRDDMLVWPWQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 257482056 | ref | ZP_05636097_1 | SLARIQT--PTLLIANRDDMLVWPWQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 289648344 | ref | ZP_06479687_1 | SLARIQT--PTLLIANRDDMLVWPWQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 320325736 | gb | EFW81797_1 | a | SLTRIQT--PTLLIANRDDMLVWPWQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 28868369 | ref | NP_790988_1 | a | QLARIQT--PTLLIANRDDMLVWPWQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
Q887X6_PESM_16-250 | QLARIQT--PTLLIANRDDMLVWPWQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 213967180 | ref | ZP_03395329_1 | QLARIQT--PTLLIANRDDMLVWPWQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 136155592 | ref | YP_002125071 | KLGKITT--PTFALANKDMLVWPWQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
B4RRW2_ALTMD_35-269 | KLGKITT--PTFALANKDMLVWPWQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 239994720 | ref | ZP_04715244_1 | RLHAITT--PTLLIANRDDMLVWPWQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 262376021 | ref | ZP_06069252_1 | EHQALKIDIPHLLANQDDFLVWPYQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
D0S49_ACILW_16-255 | EHQALKIDIPHLLANQDDFLVWPYQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 293611018 | ref | ZP_06693317_1 | EHLQALQDTHLIVANQDDFLVPAHKSODIPTKLGHQGLCLPSGASNIITDPLFPQRTLLDFLNAQT-----
gi | 262368332 | ref | ZP_06061661_1 | EIRAALQNTIPMHLIANQDDFLVWPYQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
D0S9G1_ACIO_16-250 | EIRAALQNTIPMHLIANQDDFLVWPYQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 50083320 | ref | YP_044830_1 | a | ARIDTLKQLPVCLIANQDDFLVWPYQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
Q6FFZ9_ACIA_16-255 | ARIDTLKQLPVCLIANQDDFLVWPYQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 255319344 | ref | ZP_05360561_1 | VARQIQN--PTLVLTNQDDFLVWPYQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
C6RN00_ACIRA_16-250 | VARQIQN--PTLVLTNQDDFLVWPYQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
D0T3M4_ACIRA_16-250 | VARQIQN--PTLVLTNQDDFLVWPYQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 316935661 | ref | YP_004110643 | RLDEIRH--STLVASAKDDFLVWPYQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
D2MBB4_RHOPA_24-258 | RLDEIRH--STLVASAKDDFLVWPYQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 159185242 | ref | NP_355444_2 | RLGEIGN--PVLVATKDDLLVPPYTRSLRLAEBGLPQSELCLLDFGASNIITDPLFPQRTLLDFLNAQT-----
Q7CW3_AGR75_16-250 | RLGEIGN--PVLVATKDDLLVPPYTRSLRLAEBGLPQSELCLLDFGASNIITDPLFPQRTLLDFLNAQT-----
gi | 222080882 | ref | YP_002540245 | RLSEIRT--PTLVVTRDDLLVPPYTRSLRLAEBGLPQSELCLLDFGASNIITDPLFPQRTLLDFLNAQT-----
B9UL76_AGRK_16-250 | RLSEIRT--PTLVVTRDDLLVPPYTRSLRLAEBGLPQSELCLLDFGASNIITDPLFPQRTLLDFLNAQT-----
gi | 239817801 | ref | YP_002946711 | RLGAITA--PTLVAAMDMLVWPYQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
C5CN82_YARPS_16-250 | RLGAITA--PTLVAAMDMLVWPYQSQHLAEALPNARLVLLLEYGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 167647941 | ref | YP_001685604 | DLLETIRC--PVLVASADDMLVPLSCSRRLAERLNATLDIAPWGGGFTVTPEAFNRAVLLDFLNAQT-----
B0S62_CAUSK_24-258 | DLLETIRC--PVLVASADDMLVPLSCSRRLAERLNATLDIAPWGGGFTVTPEAFNRAVLLDFLNAQT-----
gi | 295689471 | ref | YP_003593164 | RLEEIPH--RVLVASADDMLVPMSCSQRLLAARLPNADFPQVAVGGGFTVTPEAFNRAVLLDFLNAQT-----
D0XXH0_9CAUL_24-258 | RLEEIPH--RVLVASADDMLVPMSCSQRLLAARLPNADFPQVAVGGGFTVTPEAFNRAVLLDFLNAQT-----
gi | 16127029 | ref | NP_421593_1 | a | RLEDITH--RVLISASADDMLVPMSCSQRLLAARLPNADFPQVAVGGGFTVTPEAFNRAVLLDFLNAQT-----
B8HIQ3_CAUCN_27-261 | RLEDITH--RVLISASADDMLVPMSCSQRLLAARLPNADFPQVAVGGGFTVTPEAFNRAVLLDFLNAQT-----
Q9A4N3_CAUCN_27-261 | RLEDITH--RVLISASADDMLVPMSCSQRLLAARLPNADFPQVAVGGGFTVTPEAFNRAVLLDFLNAQT-----
gi | 170747999 | ref | YP_001754259 | RLGAIGH--ETLVMAARDMLVPPYTRSERLAALPNARLDLAPEGGASNIITDPLFPQRTLLDFLNAQT-----
B1M515_METRJ_17-251 | RLGAIGH--ETLVMAARDMLVPPYTRSERLAALPNARLDLAPEGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 218530013 | ref | YP_002420829 | ALGRIPH--ETLLMAARDMLVPPYTRSERLAALPNARLDLAPEGGASNIITDPLFPQRTLLDFLNAQT-----
B7KWT4_METC4_18-252 | ALGRIPH--ETLLMAARDMLVPPYTRSERLAALPNARLDLAPEGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 163851162 | ref | YP_001639205 | ALPRIPH--ETLLMAARDMLVPPYTRSERLAALPNARLDLAPEGGASNIITDPLFPQRTLLDFLNAQT-----
A9W3H8_METEP_18-252 | ALPRIPH--ETLLMAARDMLVPPYTRSERLAALPNARLDLAPEGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 240138315 | ref | YP_002962787 | ALGRIPH--ETLLMAARDMLVPPYTRSERLAALPNARLDLAPEGGASNIITDPLFPQRTLLDFLNAQT-----
C5B0U6_METEA_18-252 | ALGRIPH--ETLLMAARDMLVPPYTRSERLAALPNARLDLAPEGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 254560857 | ref | YP_003067952 | ALARIPH--ETLLMAARDMLVPPYTRSERLAALPNARLDLAPEGGASNIITDPLFPQRTLLDFLNAQT-----
C7CM33_METED_18-252 | ALARIPH--ETLLMAARDMLVPPYTRSERLAALPNARLDLAPEGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 188580343 | ref | YP_001923788 | ALARIPH--ETLLMAARDMLVPPYTRSERLAALPNARLDLAPEGGASNIITDPLFPQRTLLDFLNAQT-----
B1ZB18_METPB_18-252 | ALARIPH--ETLLMAARDMLVPPYTRSERLAALPNARLDLAPEGGASNIITDPLFPQRTLLDFLNAQT-----
gi | 158424120 | ref | YP_001525412 | RLADIRV--PTLLAAAKDDMLVPSYSLTLLAEGIPDARIAEVDWGAASNIITDPLFPQRTLLDFLNAQT-----
A8IAD8_AZOC5_22-255 | RLADIRV--PTLLAAAKDDMLVPSYSLTLLAEGIPDARIAEVDWGAASNIITDPLFPQRTLLDFLNAQT-----

Fig S2. Two-dimensional projection of the CLANS clustering results obtained for the α/β hydrolase_6 sequences. Proteins are indicated by dots, and clusters are circled and labeled according to their membership in different families. Lines indicate sequence similarity as reported by BLAST and are colored in shades of grey according to the BLAST P-value. The diagram shows 14000 sequences remaining after initial clustering and is zoomed in on the RutD and PcaD clusters.

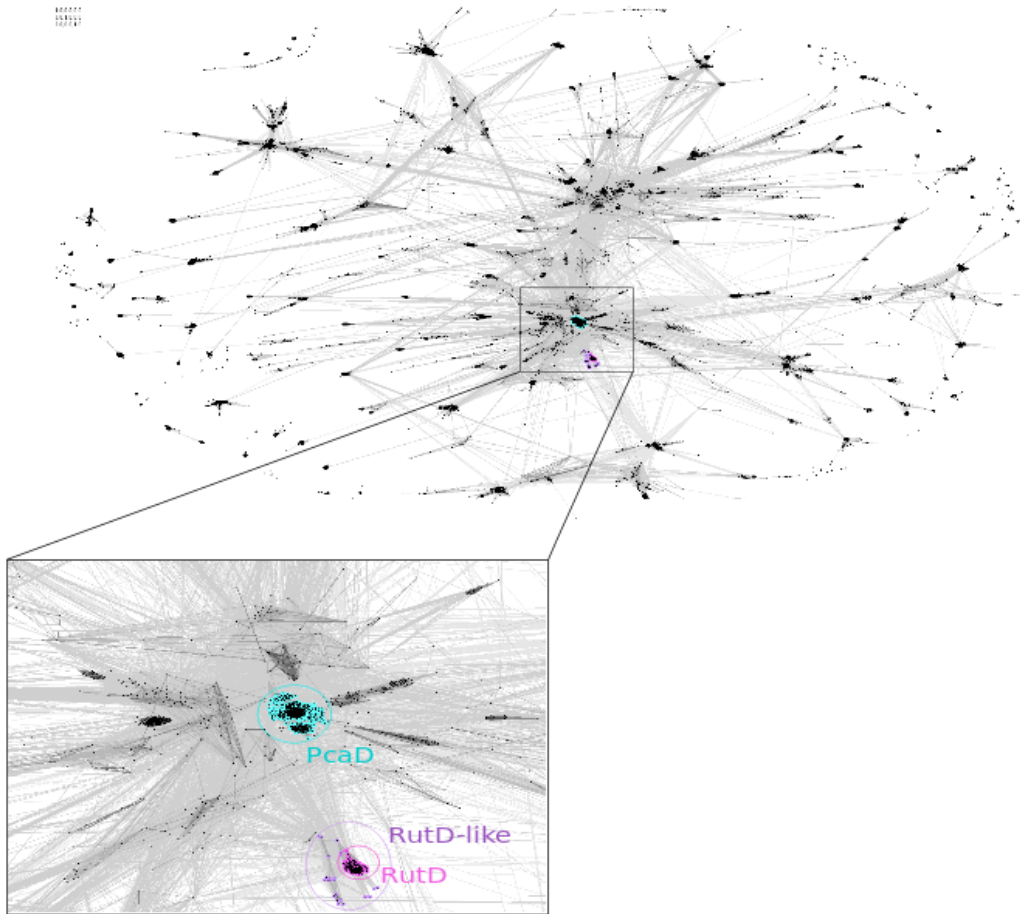


Fig.S3. Diffraction image of RutD crystal. Image shows presence of multiple crystal lattices.

